

Analytic structure of one-loop coefficients

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ABSTRACT: By the unitarity cut method, analytic expressions of one-loop coefficients have been given in spinor forms. In this paper, we present one-loop coefficients of various bases in Lorentz-invariant contraction forms of external momenta. Using these forms, the analytic structure of these coefficients becomes manifest. Firstly, coefficients of bases contain only second-type singularities while the first-type singularities are included inside scalar bases. Secondly, the highest degree of each singularity is correlated with the degree of the inner momentum in the numerator. Thirdly, the same singularities will appear in different coefficients, thus our explicit results could be used to provide a clear physical picture under various limits (such as soft or collinear limits) when combining contributions from all bases.

KEYWORDS: Analytic structure, one-loop coefficients.

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1. Introduction

In the last ten years, enormous progresses have been made in the computation of scattering amplitudes at both tree-level (see [1, 2]) and one-loop level (see, for example, the reference [3, 4, 5] and citations in the paper). All these progresses come out as a better understanding of the analytic structure of scattering amplitudes at various orders.

At the tree-level, the analytic structure is relatively simple: there is only the single-pole structure. However, even with the single-pole structure, since there are many kinematic variables, we are facing the multi-variable complex analysis as shown in the old S-matrix program [6], whose central theme is to determining scattering amplitudes directly from their analytic structures. This complicated mathematical problem is avoided in the BCFW on-shell recursion relations [7, 8, 9, 10, 11, 12, 13], which is an outgrowth of Witten's twistor program[14, 15]. The key simplification of BCFW recursion relations is that by a proper momentum deformation of two external particles, we have reduced the multi-variable complex analysis to the single-variable complex analysis.

Using the BCFW recursion relations, we can get very compact analytical expressions of tree-level amplitudes at the price of introducing the spurious-pole structure. Although each term may contain these spurious poles, they will be canceled out after the sum of all terms, since they are not physical. Nevertheless they are crucial for simple and compact expressions and have very beautiful geometrical picture as shown in [16, 17, 18, 19].

At the one-loop level, although the integrand is still rational functions of external momenta (i.e., there is only the single-pole structure), its integral will produce the branch cut structure¹. The location of singularities of one-loop results can be determined by Landau equations [6] and these singularities can be divided into the first-type and second-type. Based on these analytic structures, a reduction method [20, 21, 22, 23] has been proposed and becomes the standard method for one-loop amplitudes. The reduction tells us that a general one-loop scattering amplitude may be expanded in terms of master integrals with rational coefficients. This expansion has split the branch cut structure into the master integrals, while rational coefficients contain the information of locations of singularities. Since the master integrals are relatively well understood [20, 21], the one-loop calculation is reduced to the computation of these coefficients of the master integrals. Based on the rational structure of one-loop integrands, the very powerful OPP method [24, 25] and Forde's methods [26, 27] have been proposed. Based on the branch cut structure, a unitarity cut method was initiated by Bern *et al* [28, 29] and was further generalized first in 4 dimensions[30, 31] and then in generalized D dimensions[32, 33, 34, 35, 36].

Although these well known analytic structures of one-loop amplitudes have led us to very powerful computation methods such as OPP method and the unitarity cut method, there are still some problems regarding the analytic structure to be solved. The first problem is that although from Landau equations we can determine the location of singularities, the degree of singularities is not fully discussed. The information of degree is very important both for theoretical study and practical calculations, such as the rational part

¹Although the branch cut can be chosen arbitrarily, the starting point (branch-point) has a definite physical meaning.

of one-loop amplitudes. The rational part will appear if the expansion master basis is the pure 4D scalar box, scalar triangle, scalar bubble or scalar tadpole. As carefully discussed in [37, 38, 39], the rational part of one-loop amplitudes contains the double pole like $\frac{1}{\langle 4|5\rangle^2}$ for $A_5(1^-, 2^+, 3^+, 4^+, 5^+)$ for the gauge theory. Thus to be able to use the recursion relation to calculate, we need to determine the degree of poles as well as their residues. Besides the degree of poles, we will meet the structure like $\frac{[a|b]}{\langle a|b\rangle}$ which is just a phase in the physical region, but a true pole in the general complex plane. The third related analytic property we would like to understand is the factorization property when $((K^2 - M^2) \rightarrow 0$. Unlike the tree-level amplitudes with the factorization property $A_n^{tree} \rightarrow A_L^{tree} A_R^{tree}$, for one-loop amplitudes, we have $A^{1-loop} \rightarrow A_L^{tree} A_R^{1-loop} + A_L^{1-loop} A_R^{tree} + \mathcal{F}$ and there is still no general theory for the structure of the extra term \mathcal{F} .

Above discussions are main motivations of our current investigation. To learn more about the analytical structure of one-loop amplitudes, it is always very helpful if we can find explicit expressions for one-loop amplitudes. With recent developments, especially the unitarity cut methods, now we are able to do so. In [34], analytic expressions for various coefficients of master integrals have been given in the spinor forms. However from the spinor forms it is hard to read out analytic properties, thus the first step toward a better understanding is to translate the spinor form into the Lorentz-invariant contraction of external momenta.

After the coefficients are written in manifestly Lorentz-invariant forms, many analytic properties become obvious. The old analysis made in [6] tells that singularities can be divided into the first-type and the second-type. The first-type singularities are fully determined by the dual diagrams and all occur in the scalar bases (master integrals) which are well understood. For the second-type singularities, our results seem to indicate that they appear only in coefficients of bases. Although it is well known that the second-type singularities depend on the dimensionality of space-time, the spins of particles, and the details of the their interactions [40], their dependence is not fully discussed. The main reason is that given the topology of Feynman diagrams, the denominator of integrand is determined while the numerator can be arbitrary. In fact, it is the detail of the numerator that defines the theory under consideration. With our general explicit results presented in this paper, we are able to have a better understanding of dependence of the analytic structure on numerators. For example, the degree of second-type singularities appearing in triangle and bubble coefficients will correlate with the degree of the internal momentum $\tilde{\ell}$ in the numerator. This is one new result coming out from our analysis.

Having analytic expressions for coefficients will open a door for other analysis. Just like the tree-level BCFW recursion relations, we can take pair of momenta to make the deformation, thus reduce the multi-variable complex analysis to the single-variable complex analysis. The hope is that with these understanding, one can find similar recursion relations for one-loop coefficients. Furthermore, the Lorentz-invariant forms of one-loop coefficients are also the preparations for two-loop calculations² using the unitarity cut method.

We must emphasize that although our final goal is to address above problems, the result in this paper

²Recent new techniques for amplitude calculations at two- and higher-loop can be found in [41, 42, 43, 44, 45].

is just the first step toward this goal and there are still a lot more to be done in future. Thus our results are purely theoretical orientated and there is nothing to do with improving the efficiency of current powerful methods for one-loop calculations.

Having above motivations in the mind, in this paper, we show how to transform the spinor form of one-loop coefficients into the Lorentz-invariant forms. The evaluation is done within the spinor formalism [46], reviewed in [47]. Using these Lorentz invariant forms, we further discuss the analytic structures of coefficients, with some clarifications and interpretations using the S-matrix theory [6].

The outline of this paper is as follows. In section 2, we give a brief review of the D -dimensional unitarity cut method and the derivation of the one-loop coefficients. At same time, some conventions and notations are set up. In section 3, some knowledge about Landau equations and singularities of S-matrix programm are reviewed. This section is important to understand our results. In section 4, we transform the spinor forms of pentagon and box coefficients into the Lorentz-invariant forms. To enable readers to grasp main points of our calculations, we have summarized the result in the first subsection 4.1 and leave the details of derivations in later subsections. We do similar organizations in section 5 and 6 for triangle and bubble coefficients respectively. Finally in the conclusion section, we summarize main points of the paper and have several discussions regarding various possible further applications and clarifications. In Appendix A, an typical formula, which is important in the process from the spinor form to the Lorentz-invariant form, is given with the proof.

2. Setup

In this section, we briefly review the $(4 - 2\epsilon)$ -dimensional Unitarity method [32, 33] and the derivation of one-loop coefficients [34, 35, 36, 48], which are the foundation of our work. In this process, we also set up some key conventions and notations for latter calculations. Here we use the QCD convention for the square bracket $[i\ j]$, so that $2k_i \cdot k_j = \langle i\ j \rangle [j\ i]$.

2.1 Unitarity cut method

The unitarity cut of a one-loop amplitude is its discontinuity across a branch cut in a kinematic region selecting a particular momentum channel. By denoting the momentum vector across the cut as K , the discontinuity for a double cut can be written as

$$C = -i(4\pi)^{D/2} \int \frac{d^D p}{(2\pi)^D} \delta^{(+)}(p^2 - M_1^2) \delta^{(+)}((p - K)^2 - M_2^2) \mathcal{T}(p), \quad (2.1)$$

where

$$\mathcal{T}(p) = A_{\text{Left}}^{\text{tree}}(p) \times A_{\text{Right}}^{\text{tree}}(p). \quad (2.2)$$

The $\mathcal{T}(p)$ can be calculated by any method, for example Feynman diagrams, off-shell recursion relations [49] or BCFW on-shell recursion relations [7, 8].

The "unitarity cut method" combines the unitarity cuts with the familiar PV-reduction method [22]. PV-reduction tells us that any one-loop amplitude can be expanded in master integrals I_i

$$A^{1-loop} = \sum_i c_i I_i. \quad (2.3)$$

The master integrals in $(4 - 2\epsilon)$ -dimensions are tadpoles, bubbles, triangles, boxes and pentagons³. It is worth to emphasize that the basis includes the dimensional-shifted basis [51]. More explicitly, if we split the $(4 - 2\epsilon)$ -dimensional internal momentum $p = p_4 + \mu$ with p_4 the component in the 4D and μ the component in the (-2ϵ) -dimension, then the basis include the one like

$$I_m^D[(\mu^2)^r] \equiv i(-)^{m+1}(4\pi)^{D/2} \int \frac{d^4 p_4}{(2\pi)^4} \frac{d^{-2\epsilon} \mu}{(2\pi)^{-2\epsilon}} \frac{(\mu^2)^r}{(p^2 - \mu^2) \dots ((p - \sum_{i=1}^{m-1} K_i)^2 - \mu^2)} \quad (2.4)$$

$I_m^D[(\mu^2)^r]$ can be translated into the scalar basis with dimensional shifting as

$$I_m^{D=4-2\epsilon}[(\mu^2)^r] = -\epsilon(1-\epsilon)\dots(r-1-\epsilon)I_m^{D=4+2r-2\epsilon}[1] \quad (2.5)$$

It is, in fact, coefficients of these dimensional shifted bases producing the rational part of one-loop amplitudes mentioned in the introduction. To see it, let us notice that, for example [52],

$$\begin{aligned} \int d^{4-2\epsilon} p \frac{\mu^2}{D_i D_j} &= -\frac{i\pi^2}{2} \left[m_i^2 + m_j^2 - \frac{(p_i - p_j)^2}{3} \right] + \mathcal{O}(\epsilon) \\ \int d^{4-2\epsilon} p \frac{\mu^2}{D_i D_j D_k} &= -\frac{i\pi^2}{2} + \mathcal{O}(\epsilon) \\ \int d^{4-2\epsilon} p \frac{\mu^4}{D_i D_j D_k D_l} &= -\frac{i\pi^2}{6} + \mathcal{O}(\epsilon) \\ \int d^{4-2\epsilon} p \frac{\mu^2 q^\mu}{D_i D_j D_k} &= +\frac{i\pi^2}{6} (p_i + p_j + p_k)^\mu + \mathcal{O}(\epsilon) \\ \int d^{4-2\epsilon} p \frac{\mu^2 q^\mu q^\nu}{D_i D_j D_k D_l} &= -\frac{i\pi^2}{12} g^{\mu\nu} + \mathcal{O}(\epsilon) \end{aligned} \quad (2.6)$$

where $D_i \equiv (p + p_i)^2 - m_i^2$.

In the unitarity cut method, we derive the coefficient by performing unitarity cuts on both sides of Eq.(2.3):

$$\Delta A^{1-loop} = \sum_i c_i \Delta I_i. \quad (2.7)$$

If we can calculate the left-hand side, by comparison, we can read out the wanted coefficients c_i at the right-hand side.

³For massless external particles, tadpoles do not show up. If we constraint to pure 4D case, pentagons will not show up, but rational terms appear.

The $(4 - 2\epsilon)$ -dimensional Lorentz-invariant phase-space (LIPS) of a double cut is defined by inserting two δ -functions representing the cut conditions:

$$\int d^{4-2\epsilon} p \delta^{(+)}(p^2 - M_1^2) \delta^{(+)}((p - K)^2 - M_2^2) \quad (2.8)$$

To simplify LIPS, we can decompose $(4 - 2\epsilon)$ -dimensional momentum p as

$$p = \tilde{\ell} + \vec{\mu}; \quad \int d^{4-2\epsilon} p = \int d^{-2\epsilon} \mu \int d^4 \tilde{\ell}, \quad (2.9)$$

where $\tilde{\ell}$ belongs to 4-dimensional part and $\vec{\mu}$, (-2ϵ) -dimensional part. The 4D part momentum $\tilde{\ell}$ can be further decomposed as

$$\tilde{\ell} = \ell + zK, \quad \ell^2 = 0; \quad \int d^4 \tilde{\ell} = \int dz d^4 \ell \delta^{(+)}(\ell^2) (2\ell \cdot K), \quad (2.10)$$

where K is the pure 4D cut momentum and ℓ is pure 4D massless momentum, which can be expressed with spinor variables as

$$\ell = t P_{\lambda\tilde{\lambda}}, \quad P_{\lambda\tilde{\lambda}} = \lambda\tilde{\lambda} = |\ell\rangle [\ell]; \quad \int d^4 \ell \delta^{(+)}(\ell^2) = \int \langle \ell d\ell \rangle [\ell d\ell] \int t dt. \quad (2.11)$$

Under this decomposing procedure, Eq.(2.8) becomes

$$\begin{aligned} \int d^{4-2\epsilon} \Phi &= \frac{(4\pi)^\epsilon}{\Gamma(-\epsilon)} \int d\mu^2 (\mu^2)^{-1-\epsilon} \int d^4 \tilde{\ell} \delta^{(+)}(\tilde{\ell}^2 - \mu^2 - M_1^2) \delta^{(+)}((\tilde{\ell} - K)^2 - \mu^2 - M_2^2) \\ &= \frac{(4\pi)^\epsilon}{\Gamma(-\epsilon)} \int d\mu^2 (\mu^2)^{-1-\epsilon} \int \langle \ell d\ell \rangle [\ell d\ell] \frac{(1 - 2z)K^2 + M_1^2 - M_2^2}{\langle \ell | K | \ell \rangle^2} \end{aligned} \quad (2.12)$$

where we have used δ -functions to solve parameters t and z as

$$t = \frac{(1 - 2z)K^2 + M_1^2 - M_2^2}{\langle \ell | K | \ell \rangle}, \quad z = \frac{(K^2 + M_1^2 - M_2^2) - \sqrt{\Delta[K, M_1, M_2] - 4K^2\mu^2}}{2K^2}, \quad (2.13)$$

with the definition

$$\begin{aligned} \Delta[K, M_1, M_2] &\equiv (K^2 - M_1^2 - M_2^2)^2 - 4M_1^2 M_2^2 \\ &= -4M_1^2 M_2^2 \left| \begin{array}{cc} 1 & -\frac{K^2 - M_1^2 - M_2^2}{2M_1 M_2} \\ -\frac{K^2 - M_1^2 - M_2^2}{2M_1 M_2} & 1 \end{array} \right|. \end{aligned} \quad (2.14)$$

For convenience, the μ^2 -integral measure can be redefined as

$$\int d\mu^2 (\mu^2)^{-1-\epsilon} = \left(\frac{\Delta[K, M_1, M_2]}{4K^2} \right)^{-\epsilon} \int_0^1 du u^{-1-\epsilon},$$

where the relation between u and μ^2 is given by

$$u \equiv \frac{4K^2 \mu^2}{\Delta[K, M_1, M_2]}. \quad (2.15)$$

Using the new variable u , we can rewrite z, t as

$$z = \frac{\alpha - \beta\sqrt{1-u}}{2}, \quad t = \beta\sqrt{1-u} \frac{K^2}{\langle \ell|K|\ell \rangle}, \quad (2.16)$$

where

$$\alpha = \frac{K^2 + M_1^2 - M_2^2}{K^2}, \quad \beta = \frac{\sqrt{\Delta[K, M_1, M_2]}}{K^2}. \quad (2.17)$$

Putting all together, the cut integral Eq.(2.1) is transformed to

$$C = \frac{(4\pi)^\epsilon}{i\pi^{D/2}\Gamma(-\epsilon)} \left(\frac{\Delta[K, M_1, M_2]}{4K^2} \right)^{-\epsilon} \int_0^1 du u^{-1-\epsilon} \\ \times \int \langle \ell d\ell \rangle [\ell d\ell] \beta\sqrt{1-u} \frac{K^2}{\langle \ell|K|\ell \rangle^2} \mathcal{T}(p). \quad (2.18)$$

where $\mathcal{T}(p)$ should be interpreted as

$$\mathcal{T}(p) = \mathcal{T}(\tilde{\ell}, \mu^2) = \mathcal{T}(tP_{\lambda\tilde{\lambda}} + zK, \mu^2) = \mathcal{T}(|\ell|, |\ell|, \mu^2), \quad (2.19)$$

with

$$\tilde{\ell} = tP_{\lambda\tilde{\lambda}} + zK = \frac{K^2}{\langle \ell|K|\ell \rangle} \left[\beta \left(P_{\lambda\tilde{\lambda}} - \frac{K \cdot P_{\lambda\tilde{\lambda}}}{K^2} K \right) + \alpha \frac{K \cdot P_{\lambda\tilde{\lambda}}}{K^2} K \right]. \quad (2.20)$$

2.2 Input

For standard quantum field theory⁴, $\mathcal{T}(p)$ is always a sum of following terms⁵

$$\mathcal{T}(\tilde{\ell}) = \frac{\prod_{j=1}^{n+k} (2\tilde{\ell} \cdot R_j)}{\prod_{i=1}^k ((\tilde{\ell} - K_i)^2 - m_i^2 - \mu^2)}. \quad (2.21)$$

The number of propagators is given by k , thus to have triangles in the expansion, we need to have $k \geq 1$. To have boxes, $k \geq 2$ and pentagons $k \geq 3$. The degree of $\tilde{\ell}$ in numerator is given by $n+k$, so we require $n+k \geq 0$ only.

If we define

$$\tilde{R} = \sum_{j=1}^{n+k} x_j R_j, \quad (2.22)$$

then $\prod_{j=1}^{n+k} (2\tilde{\ell} \cdot R_j)$ is just the $\prod_{j=1}^{n+k} x_j$ - component after expanding $(2\tilde{\ell} \cdot \tilde{R})^{n+k}$. So, for simplicity of our general discussions, we just need take the following form as the input:

$$\mathcal{T}(\tilde{\ell}) = \frac{(2\tilde{\ell} \cdot \tilde{R})^{n+k}}{\prod_{i=1}^k ((\tilde{\ell} - K_i)^2 - m_i^2 - \mu^2)}. \quad (2.23)$$

⁴For non-local theories or some effective theories, the assumption of input in (2.21) is not right.

⁵Since all external momenta are in pure 4D, the contributions of p in $(4-2\epsilon)$ -dimension can only have either μ^2 -combination or $\tilde{\ell} \cdot R_j$ -combination.

According to the simplified phase-space integration Eq.(2.18), the cut integral can be written as

$$C = \frac{(4\pi)^\epsilon}{i\pi^{D/2}\Gamma(-\epsilon)} \left(\frac{\Delta[K, M_1, M_2]}{4K^2} \right)^{-\epsilon} \int_0^1 du u^{-1-\epsilon} \\ \times \int \langle \ell d\ell \rangle [\ell d\ell] \beta \sqrt{1-u} \frac{(K^2)^{n+1}}{\langle \ell | K | \ell \rangle^{n+2}} \frac{\langle \ell | R | \ell \rangle^{n+k}}{\prod_{i=1}^k \langle \ell | Q_i | \ell \rangle}. \quad (2.24)$$

In the above equation,

$$R = \beta(\sqrt{1-u})r + \alpha_R K, \quad Q_i = \beta(\sqrt{1-u})q_i + \alpha_i K \quad (2.25)$$

where

$$r = \tilde{R} - \frac{\tilde{R} \cdot K}{K^2} K, \quad \alpha_R = \alpha \frac{\tilde{R} \cdot K}{K^2} \\ q_i = K_i - \frac{K_i \cdot K}{K^2} K, \quad \alpha_i = \alpha \frac{K_i \cdot K}{K^2} - \frac{K_i^2 + M_1^2 - m_i^2}{K^2}. \quad (2.26)$$

For the integrand

$$I = \frac{(K^2)^{n+1}}{\langle \ell | K | \ell \rangle^{n+2}} \frac{\langle \ell | R | \ell \rangle^{n+k}}{\prod_{i=1}^k \langle \ell | Q_i | \ell \rangle}, \quad (2.27)$$

based on spinor formalism, it can be split into

$$I = \sum_{i=1}^k F_i(\ell) \frac{1}{\langle \ell | K | \ell \rangle \langle \ell | Q_i | \ell \rangle} + \sum_{q=0}^n G_q(\ell) \frac{\langle \ell | R | \ell \rangle^q}{\langle \ell | K | \ell \rangle^{q+2}}, \quad (2.28)$$

where

$$F_i(\ell) = \frac{(K^2)^{n+1}}{\langle \ell | K Q_i | \ell \rangle^{n+1}} \frac{\langle \ell | R Q_i | \ell \rangle^{n+k}}{\prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle}, \quad (2.29)$$

$$G_q(\ell) = \sum_{i=1}^k \frac{(K^2)^{n+1} \langle \ell | R Q_i | \ell \rangle^{n-q+k-1} \langle \ell | K R | \ell \rangle}{\langle \ell | K Q_i | \ell \rangle^{n-q+1} \prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle}. \quad (2.30)$$

The F_i term contributes to pentagon, boxes and triangles, while the G_q term, bubbles. Substituting the splitting result into Eq.(2.24), and taking the residues of different poles, we can get coefficients of various master integrals. Notice that the value of n constrains the basis of master integrals. Terms with $n \leq -2$ contribute only to boxes and pentagons, and those with $n \geq -1$ contribute to triangles in addition. If $n \geq 0$, contributions to bubbles will kick in. For renormalizable theory, we have $n \leq 2$. However, in this paper, our discussion adapts to an arbitrary n , such as gravity theory.

2.3 Summary of coefficients

Now we list the coefficients of different master integrals. The pentagon and box coefficients are given by

$$C[Q_i, Q_j, K] = \frac{(K^2)^{n+2}}{2} \left(\frac{\langle P_{ij,1} | R | P_{ij,2} \rangle^{n+k}}{\langle P_{ij,1} | K | P_{ij,2} \rangle^{n+2} \prod_{t=1, t \neq i, j}^k \langle P_{ij,1} | Q_t | P_{ij,2} \rangle} + \{P_{ij,1} \rightarrow P_{ij,2}\} \right) \quad (2.31)$$

where $P_{ij,1}$ and $P_{ij,2}$ are two null momenta constructed from Q_i and Q_j ($i \leq j$). More explicitly, if both Q_i, Q_j are massless, then we can set $Q_i = P_{ij,1}$ and $Q_j = P_{ij,2}$. If one of them is not massless, for example, $Q_i^2 \neq 0$, we can construct

$$P_{ij} = (Q_j + xQ_i) \quad . \quad (2.32)$$

The condition $P_{ij}^2 = 0$ leads to following two solutions of x

$$x_{1,2} = \frac{-2Q_i \cdot Q_j \pm \sqrt{(2Q_i \cdot Q_j)^2 - 4Q_i^2 Q_j^2}}{2Q_i^2}, \quad (2.33)$$

thus we have constructed two null momenta. Formula (2.31) makes sense when and only when $k \geq 2$. Furthermore, if $n \leq -3$ (noticing that we need to have $n + k \geq 0$), there is only pentagon coefficients.

The triangle coefficient is given by

$$C[Q_i, K] = \frac{(K^2)^{n+1}}{2} \frac{1}{(\sqrt{\Delta})^{n+1}} \frac{1}{(n+1)! \langle P_{i,1} | P_{i,2} \rangle^{n+1}} \times \frac{d^{n+1}}{d\tau^{n+1}} \left(\frac{\langle \ell | R Q_i | \ell \rangle^{n+k}}{\prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \Big|_{\ell \rightarrow P_{i,1} - \tau P_{i,2}} + \{P_{i,1} \leftrightarrow P_{i,2}\} \right) \Big|_{\tau \rightarrow 0} \quad (2.34)$$

where $P_{i,1}$ and $P_{i,2}$ are two null momentum constructed from K and Q_i . Formula (2.34) makes sense when and only when $k \geq 1$ and $n \geq -1$.

The coefficient of the bubble is the sum of the residues of the poles from the following expression:

$$B = \sum_{i=1}^k \sum_{q=0}^n \frac{-(K^2)^{n+1} \langle \ell | R Q_i | \ell \rangle^{n-q+k-1}}{\langle \ell | K Q_i | \ell \rangle^{n-q+1} \prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \frac{1}{q+1} \frac{\langle \ell | R | \ell \rangle^{q+1}}{\langle \ell | K | \ell \rangle^{q+1}} \quad (2.35)$$

where poles are given by factors $\langle \ell | K Q_i | \ell \rangle$ and $\langle \ell | Q_t Q_i | \ell \rangle$. Formula (2.35) makes sense when and only when $k \geq 0$ and $n \geq 0$.

2.4 Notations

For convenience, we give notations we will adopt in the paper. First we define the following determinant

$$G \begin{pmatrix} p_1 & p_2 & \cdots & p_k \\ q_1 & q_2 & \cdots & q_k \end{pmatrix} = \det (p_i \cdot q_j)_{k \times k}. \quad (2.36)$$

If $q_i = p_i$ we write

$$G(p_1, p_2, \dots, p_k) \equiv G \begin{pmatrix} p_1 & p_2 & \dots & p_k \\ p_1 & p_2 & \dots & p_k \end{pmatrix}. \quad (2.37)$$

If $q_i = p_i$ for $i = 1, \dots, k-1$ in (2.36), for short we can write it as

$$(p_k | q_k) |_{p_1, \dots, p_{k-1}} = G \begin{pmatrix} p_1 & p_2 & \dots & p_{k-1} & p_k \\ p_1 & p_2 & \dots & p_{k-1} & q_k \end{pmatrix}. \quad (2.38)$$

If the meaning of p_1, \dots, p_{k-1} is unambiguous, we can even write it as $(p_k | q_k)$.

Second we define other determinants which are related to the Gram determinant, but depend on the masses of propagators. They are

$$N^{(K_i, K_j, K; \tilde{R})} = -\det \begin{pmatrix} 0 & K^2 + M_1^2 - M_2^2 & K_i^2 + M_1^2 - m_i^2 & K_j^2 + M_1^2 - m_j^2 \\ \tilde{R} \cdot K & K^2 & K_i \cdot K & K_j \cdot K \\ \tilde{R} \cdot K_i & K \cdot K_i & K_i^2 & K_j \cdot K_i \\ \tilde{R} \cdot K_j & K \cdot K_j & K_i \cdot K_j & K_j^2 \end{pmatrix} \quad (2.39)$$

with 4 parameters and the structurally similar

$$N^{(K_i, K_j, K_t, K; \tilde{R})} = -\det \begin{pmatrix} 0 & K^2 + M_1^2 - M_2^2 & K_i^2 + M_1^2 - m_i^2 & K_j^2 + M_1^2 - m_j^2 & K_t^2 + M_1^2 - m_t^2 \\ \tilde{R} \cdot K & K^2 & K_i \cdot K & K_j \cdot K & K_t \cdot K \\ \tilde{R} \cdot K_i & K_i \cdot K & K_i^2 & K_i \cdot K_j & K_t \cdot K_i \\ \tilde{R} \cdot K_j & K_j \cdot K & K_i \cdot K_j & K_j^2 & K_t \cdot K_j \\ \tilde{R} \cdot K_t & K_t \cdot K & K_i \cdot K_t & K_j \cdot K_t & K_t^2 \end{pmatrix}. \quad (2.40)$$

with 5 parameters. Another one is

$$D^{(K_i, K_j, K_t, K_s, K)} = \det \begin{pmatrix} K^2 + M_1^2 - M_2^2 & K_i^2 + M_1^2 - m_i^2 & K_j^2 + M_1^2 - m_j^2 & K_t^2 + M_1^2 - m_t^2 & K_s^2 + M_1^2 - m_s^2 \\ K \cdot K_i & K_i^2 & K_i \cdot K_j & K_i \cdot K_t & K_i \cdot K_s \\ K \cdot K_j & K_i \cdot K_j & K_j^2 & K_t \cdot K_j & K_j \cdot K_s \\ K \cdot K_t & K_i \cdot K_t & K_t \cdot K_j & K_t^2 & K_t \cdot K_s \\ K \cdot K_s & K_i \cdot K_s & K_j \cdot K_s & K_t \cdot K_s & K_s^2 \end{pmatrix}, \quad (2.41)$$

which is related to reducing the hexagon to the pentagon.

3. Singularities

One main motivation of our calculations is to discuss the analytic structure of coefficients of master integrals. For this purpose, in this section, we will review some backgrounds coming from the study of S-matrix

program [6, 40]. The main point is that locations of all possible singularities of a Feynman integral can be determined, in principle, by the Landau equations. These singularities can be divided into two types: the first-type and the second-type. However, as we have mentioned in the introduction, the degree of singularities, especially the second-type singularities, has not been discussed in [6, 40].

3.1 Landau equations

To start, let us notice that apart from constant multiplicative factors, after Feynman parametrization, the general Feynman integral takes the form

$$I = \int \frac{\nu(q)\delta(\sum_i \alpha_i - 1) \left(\prod_{i=1}^N d\alpha_i \right) \left(\prod_{j=1}^N d^n k_j \right)}{\psi^N}, \quad (3.1)$$

with ψ defined by

$$\psi(p, k, \alpha) = \sum_{i=1}^N \alpha_i (q_i^2 - m_i^2). \quad (3.2)$$

Here N, l are, respectively, the numbers of the internal lines and the independent loops of the corresponding graph. α_i, q_i, m_i are, respectively, the Feynman integration parameter, the momentum, and the mass associated with the i th line. $\nu(q)$ is a polynomial which involves the spins of the participating particles and the details of their interactions. n is the dimensionality of Lorentz space.

The four momentum q_i in any internal line is a linear function of the circulating momenta k and the external momenta p . Therefore the quadratic form $\psi(p, k, \alpha)$ can be written as

$$\begin{aligned} \psi(p, k, \alpha) &= \sum_{i,j=1}^l a_{i,j} k_i k_j + \sum_{j=1}^l b_j k_j + c \\ &= \mathbf{k}^T \cdot \mathbf{A} \mathbf{k} - 2\mathbf{k}^T \cdot \mathbf{B} \mathbf{p} + (\mathbf{p}^T \cdot \mathbf{\Gamma} \mathbf{p} - \sigma), \end{aligned} \quad (3.3)$$

where

$$\sigma = \sum_i \alpha_i m_i^2. \quad (3.4)$$

Here, $\mathbf{A}, \mathbf{B}, \mathbf{\Gamma}$ are respectively $l \times l, l \times (E-1), (E-1) \times (E-1)$ matrices, whose elements are linear in α . E denotes the number of external lines of the diagram. k and p are column vectors in the spaces of the matrices and their elements are themselves Lorentz four-vectors.

For most discussions, $\nu(q) = 1$ for (3.1) has been assumed. It is enough for the location of singularities. Performing the integration over k in Eq.(3.1), we can get

$$I = \int \frac{C^{N-(1/2)n(l+1)} \delta(\sum_i \alpha_i - 1) \left(\prod_{i=1}^N d\alpha_i \right)}{D^{N-(1/2)nl}}, \quad (3.5)$$

where

$$C = \det(\mathbf{A}), \quad D = -(\mathbf{B}\mathbf{p})^T \cdot \mathbf{X}(\mathbf{B}\mathbf{p}) + (\mathbf{p}^T \cdot \mathbf{\Gamma}\mathbf{p} - \sigma)C, \quad (3.6)$$

with $X = \text{adj}(A)$ ⁶ and σ defined by Eq.(3.4). C is of degree l in the α and D , of degree $(l + 1)$. According to the generalized Hadamard lemma, the necessary conditions for a singularity of I are, using the representation Eq.(3.5),

$$\text{Form I :} \quad \alpha_i \frac{\partial D}{\partial \alpha_i} = 0, \quad \text{for each } i. \quad (3.7)$$

If we use the representation (3.1), the Landau equations will be given by

$$\text{Form II :} \quad \begin{cases} \alpha_i(q_i^2 - m_i^2) = 0, & \text{for each propagator } i \\ \sum_j \alpha_i q_i = 0, & \text{for each loop running by loop-momentum } k_j \end{cases} \quad (3.8)$$

In both forms (3.7) and (3.8), solution with $\alpha_i = 0$ corresponds to pinch the corresponding propagators, so for example, a box diagram will reduce to a triangle diagram. The singularity of a given graph with no $\alpha_i = 0$ (i.e., all propagators are on the mass shell) is called the "leading singularity".

A connection between these two forms can be found by noticing that an alternative expression for D is given by

$$D = CD', \quad (3.9)$$

where D' is the result of eliminating k from ψ by means of the equations

$$\frac{\partial \psi}{\partial k_j} = 0, \quad \text{for each } j. \quad (3.10)$$

In the notation of Eq.(3.3), these equations are

$$\mathbf{A}\mathbf{k} = \mathbf{B}\mathbf{p}. \quad (3.11)$$

Together with Eq.(3.3) and Eq.(3.10), we obtain the Landau equations (3.8).

$$\sum_j \alpha_i q_i = 0, \quad \text{for each } j, \quad (3.12)$$

and

$$\alpha_i(q_i^2 - m_i^2) = 0, \quad \text{for each } i, \quad (3.13)$$

where \sum_j in Eq.(3.12) denotes summation round the j th closed loop of the diagram.

⁶ X is always well defined even $\det(A) = 0$. If $\det(A) \neq 0$, we have $X = A^{-1}C$.

3.2 Singularities of the first type

The Landau equations are usually too complicated to solve algebraically. So a geometrical method, which is the so called dual diagram, have been introduced. The dual diagram is vector diagram for internal and external momenta. From dual diagrams we can read out the Landau surface where singularities of the first type may locate. For example, for bubble diagram, $\Delta[K, M_1, M_2]$ in (2.14) is nothing, but exactly the Landau surface. From this surface, we can find the location of singularities is $K^2 = (M_1 \pm M_2)^2$. The Landau surface of triangle is given by

$$\Sigma_{tri} = \begin{vmatrix} 1 & -y_{12} & -y_{13} \\ -y_{21} & 1 & -y_{23} \\ -y_{31} & -y_{32} & 1 \end{vmatrix}, \quad (3.14)$$

where $y_{ij} = y_{ji} = \frac{P_k^2 - m_i^2 - m_j^2}{2m_i m_j}$ with (i, j, k) a permutation of $(1, 2, 3)$. The m_i is the mass of the propagator q_i and P_i is the external momentum at the vertex i opposite to the propagator q_i . For the box diagram, let us denote external momenta clockwise as $P_i^2 = M_i^2$, $i = 1, 2, 3, 4$ and internal propagators clockwise as q_i with mass m_i (q_{i-1}, q_i and P_i meet at the same vertex), then the Landau surface is given by

$$\Sigma_{box} = \begin{vmatrix} 1 & -y_{12} & -y_{13} & -y_{14} \\ -y_{21} & 1 & -y_{23} & -y_{24} \\ -y_{31} & -y_{32} & 1 & -y_{34} \\ -y_{41} & -y_{42} & -y_{43} & 1 \end{vmatrix} \quad (3.15)$$

where $y_{ij} = y_{ji} = \frac{(q_i - q_j)^2 - m_i^2 - m_j^2}{2m_i m_j}$.

One important point of the Landau surfaces (3.14) and (3.15) of the first-type singularities is that they depend on masses of inner propagators.

3.3 Singularities of the second type

The conventional dual diagrams do not represent all possible solutions of the Landau equations. The extra solutions are called the second-type solutions. They correspond to rather special solutions of the Landau equations. In Eq.(3.11), if \mathbf{A} is non-singular, \mathbf{k} will have a unique solution in terms of the \mathbf{p} which will exactly correspond to the dual diagram construction. Hence second-type solutions will have to correspond to \mathbf{A} being singular, that is to the condition

$$C = \det \mathbf{A} = 0. \quad (3.16)$$

Second-type singularities can be divide into two classes, pure second-type and mixed second-type. The former, which are given by the Gram determinant equation (2.36)

$$G(p_1, \dots, p_{E-1}) = \det p_i \cdot p_j = 0, \quad i, j = 1, \dots, E-1, \quad (3.17)$$

where p_i represent any $(E - 1)$ of the E external momenta of the graph. The equation (3.17) is the condition that there be a linear combination of the vectors $p_1 \dots p_{E-1}$ equal to zero or, more generally, equal to a zero-length vector whose scalar products with p_1, \dots, p_{E-1} are zero. Detailed analysis reveals that second-type singularities stem from super pinches at infinity and correspond to infinite values for some of the components of the internal momenta in the Feynman graph.

Second-type singularities have some properties. First the curve given by (3.17) is *independent of the masses* of the internal particles. Secondly, the presence of second-type singularities involves the dimensionality of space, the spins of particles, and the details of the their interactions. For example, for pure scalar theory, i.e., $\nu(q) = 1$ in (3.1), only when $E < n$ (n is the dimension of space-time), second-type singularity exists. This result will be changed if $\nu(q)$ is nontrivial function.

In a diagram with several loops, there may be super pinches only for some of the loop momenta while the others have ordinary pinches at finite points. These singularities are called *mixed second-type singularities* and their equations will depend upon the internal masses of the lines round the loops with finite loops. In this paper, we will focus on one-loop diagrams, so we will not meet the mixed second-type singularities.

4. Coefficients of pentagon and box

Starting from this section, we will present the explicit Lorentz-invariant form of external momenta for various coefficients of master integrals. Since the transformation from the spinor form to the Lorentz-invariant form is a little bit complicated, we will summarize the main results at the beginning of each section and leave the derivation in the later part, for which readers can skip safely if they want.

The pentagon and box coefficients are given by Eq.(2.31). In subsection 4.1, we summarize our results and discuss analytic properties of pentagon and box coefficients derived from our calculations. In subsection 4.2, we discuss how to separate pentagon and box coefficients from the single expression (2.31). Then we evaluate box coefficients in subsection 4.3. To do so, we need carry out a typical sum, which is done in Appendix (see (A.1) and (A.11)). The same sum patten appears also for triangle and bubble coefficients.

4.1 The summary of main results of current section

Pentagon: First, the Lorentz-invariant forms of the pentagon coefficients defined by momenta K_i, K_j, K_t, K are

$$C[Q_i, Q_j, Q_t, K] = \left(\frac{N(K_i, K_j, K_t, K; \tilde{R})}{G(K_i, K_j, K_t, K)} \right)^{n+k} \prod_{w=1, w \neq i, j, t}^k \frac{G \left(\begin{smallmatrix} K_i & K_j & K_t & K \\ K_i & K_j & K_t & K_w \end{smallmatrix} \right)}{D(K_i, K_j, K_t, K_w, K)}, \quad (4.1)$$

where functions G, N can be found in (2.37), (2.40) and (2.41). From the expression (4.1) following analytic properties of pentagon coefficients can be read out:

- First the factor $G(K_i, K_j, K_t, K)$ is nothing, but the second-type singularity intrinsically related to pentagon topology. Furthermore, its degree is $(n + k)$, which is the degree of $\tilde{\ell}$ in numerator of the input (2.21). More explicitly, to have the pentagon in the expansion, we must have $k \geq 3$ in (2.21) and $n + k \geq 0$. If $n + k = 0$, the singularity $G(K_i, K_j, K_t, K)$ does not appear, but it will be there when $n + k \geq 1$.
- Secondly, there are singularities given by $D^{(K_i, K_j, K_t, K_\omega, K)}$. They come from the trivial reduction of the hexagon topology to the pentagon topology and depend on masses of propagators. Their dependence of masses is not like that of first-type singularities given in (2.14) for the bubble, (3.14) for the triangle and (3.15) for the box. In fact, the trivial reduction from the hexagon to the pentagon is intrinsically related to the four-dimensional space-time. Thus we guess the appearance of this type of singularities is also related to the space-time dimension.
- Thirdly, $C[Q_i, Q_j, Q_t, K]$ does not contain u at all. In other words, dimensional shifted bases exist only for box, triangle, bubble and tadpole topologies. This is tightly related to $(4 - 2\epsilon)$ -dimensional analysis. In fact, it is well known that if we do reduction in pure 4-dimension, the pentagon will not be a basis at all.

It is worth to point out that since the (4.1) is given by only one term, we will not expect cancelation of any factor in denominators⁷.

Box: The true box coefficients are given by

$$\begin{aligned}
C[Q_i, Q_j, K] = & \sum_{z_1 + \dots + z_k + s = n + 2} \sum_{h=0}^s \left(\prod_{t=1, t \neq i, j}^k \frac{G \left(\begin{smallmatrix} K_i & K_j & K_t & K \\ K_i & K_j & \tilde{R} & K \end{smallmatrix} \right)}{G(K_i, K_j, K_t, K)} \left(\frac{N^{(K_i, K_j, K_t, K; \tilde{R})}}{G(K_i, K_j, K_t, K)} \right)^{z_t} \right) \\
& \times \binom{s}{h} \frac{N^{(K_i, K_j, K; \tilde{R})} s^{-h} T(h)}{(G(K_i, K_j, K))^s}; \quad \text{with } h \text{ even}
\end{aligned} \tag{4.2}$$

where $T(h)$ is defined in Eq.(4.21) and G, N can be found in (2.37), (2.40). The derivation of (4.2) is given in later subsections.

Now the analytic properties of box coefficients can be read out:

⁷It is worth to emphasize that in this paper we will not discuss the cancelation of singularities after summing over contributions from all bases. For example, it is very possible that the singularity like $D^{(K_i, K_j, K_t, K_\omega, K)}$ will be canceled out if we sum up contributions from all pentagons.

- First we notice that although there are first-type and second-type singularities in general, the box coefficient contains only second-type singularities. The first-type singularity of the box appears only in the box scalar basis⁸.
- Among all second-type singularities, the one given by $G(K_i, K_j, K)$ is intrinsically related to the box topology. Among all terms of (4.2), there is one and only one term with the highest $s = n + 2$ and all other $z_t = 0$. Thus this term can not be canceled by others and the highest degree of singularity $G(K_i, K_j, K)$ is $(n + 2)$.

It is worth to compare the degree of singularities between the pentagon and the box. The highest degree of the pentagon singularity is $(n + k)$ (i.e., the degree of $\tilde{\ell}$ in the numerator) while that of the box singularity is $(n + 2)$. Naively, when we do the reduction, one $\tilde{\ell}$ in numerator will cancel one propagator, thus for box we need to cancel $(k - 2)$ propagators, so the remaining degree of $\tilde{\ell}$ in the numerator is $(n + k) - (k - 2) = (n + 2)$ as we expect. However, the degree of the pentagon singularity does not follow the rule. We think the reason is following. The naive observation is based on the reduction in 4D. If we do everything in pure 4D, the pentagon will not be a basis as given in [50]⁹,

$$I_5^{D=4-2\epsilon}[1] = \sum_{i=1}^5 c_i I_{4,i}^{D=4-2\epsilon}[1] + \epsilon I_5^{D=6-2\epsilon}[1] \quad (4.3)$$

where $I_5^{D=6-2\epsilon}[1]$ is finite when $\epsilon \rightarrow 0$. In fact, it is because we do reduction in $(4 - 2\epsilon)$ -dimension, the pentagon becomes a necessary basis. Based on the observation, we think the naive observation is not applicable to the pentagon topology and each $\tilde{\ell}$ in the numerator does give a contribution to the degree of the singularity.

- The appearance of the second-type singularity $G(K_i, K_j, K_t, K)$ indicates the influence of pentagon topologies, which will produce the same box topology when pinching one propagator. Just like the previous item, for a given singularity $G(K_i, K_j, K_t, K)$ there is one and only one term inside (4.2) with the highest degree $(n + 3)$, thus it can not be canceled by other terms. The highest degree $(n + 3)$ of the pole $G(K_i, K_j, K_t, K)$ can be understood by the naive observation, i.e., in the reduction one $\tilde{\ell}$ in the numerator will cancel one propagator. To produce the pentagon topology, we need to get rid

⁸It is shown in [40] that for 4D, the scalar box basis does not contain the second-type singularity in *physical sheet*. However, second-type singularities do appear for scalar triangle and bubble bases in 4D. The general condition is that $E < D$ where E is the number of external lines and D , dimensions of space-time. It is worth to emphasize that although second-type singularity of box does not show up in the physical sheet, it does show up in other sheet. Thus its understanding is also important for the study of analytic properties.

⁹With formula (4.3), we can change the choice of basis from $I_5^{D=4-2\epsilon}[1]$ to $I_5^{D=6-2\epsilon}[1]$. In this paper, we will choose $I_5^{D=4-2\epsilon}[1]$ as our basis to do the PV-reduction. One of the reason is that with this choice of basis, the pentagon coefficient will not depend on u , thus contributions to one-loop rational part will be contained completely in the box, triangle and bubble parts.

of $(k - 3)$ propagators, thus the degree of $\tilde{\ell}$ in the numerator becomes $(n + k) - (k - 3) = (n + 3)$. Each remaining $\tilde{\ell}$ will produce one $G(K_i, K_j, K_t, K)$ singularity when pinched to box.

- To see the dimensional shifted basis (which is related to rational part of one-loop amplitudes, see (2.4), (2.6)), we need to check the u -dependence part in the numerator. From (4.2), all u -dependence comes from the factor $T(h)$ and the highest degree of u is $[(n + 2)/2]$. It is also important to notice that each u will be accompanied by a factor $G(K_i, K_j, K)$ (see Eq.(4.21), which will reduce the highest degree of the pole $G(K_i, K_j, K)$ for these (rational) terms.

4.2 The separation of coefficients of pentagon and box

Since the expression (2.31) contains both pentagon and box coefficients, the first step is to separate the pentagon coefficient from the box. This separation has been discussed in [48]. However, since we need write them more compactly and systematically and we are dealing with the $(4 - 2\epsilon)$ -dimensional massive case, which is different from the massless case in [48], we will give the main steps to write out our results and leave some details to be referred to [48].

Expanding numerator: The first preparation for the separation is to expand r (see (2.26)) in the basis q_i, q_j, q_t as (remembering $r \cdot K = 0$)

$$r = a_t^{(q_i, q_j, q_t; r)} q_t + a_i^{(q_i, q_j, q_t; r)} q_i + a_j^{(q_i, q_j, q_t; r)} q_j, \quad (4.4)$$

which is equal to the expansion of \tilde{R} in the basis K_i, K_j, K_t, K because $q_i \cdot K = 0$:

$$\tilde{R} = a_t^{(K_i, K_j, K_t, K; \tilde{R})} K_t + a_i^{(K_i, K_j, K_t, K; \tilde{R})} K_i + a_j^{(K_i, K_j, K_t, K; \tilde{R})} K_j + a_K^{(K_i, K_j, K_t, K; \tilde{R})} K. \quad (4.5)$$

By projecting Eq.(4.5) onto the vectorspace orthogonal to K , we can easily check:

$$a_\omega^{(q_i, q_j, q_t; r)} = a_\omega^{(K_i, K_j, K_t, K; \tilde{R})}, \quad \omega = i, j, t. \quad (4.6)$$

The Crammer rule gives the solution of Eq. (4.4)

$$a_\omega^{(q_i, q_j, q_t; r)} = \frac{G \begin{pmatrix} K_i & \dots & \tilde{R} & \dots & K \\ K_i & \dots & K_\omega & \dots & K \end{pmatrix}}{G(K_i, K_j, K_t, K)}, \quad \omega = i, j, t \quad (4.7)$$

using the notation (2.36). The denominator $G(K_i, K_j, K_t, K)$ is nothing, but the *second-type singularity* related to the pentagon determined by momenta K, K_i, K_j, K_t . In other words, it can be considered as the "finger print" of the related pentagon.

Using the expansion Eq. (4.4), we have

$$\langle P_1 | R | P_2 \rangle = a_t^{(q_i, q_j, q_t; r)} \langle P_1 | Q_t | P_2 \rangle + \beta^{(q_i, q_j, q_t; r)} \langle P_1 | K | P_2 \rangle, \quad (4.8)$$

with

$$\beta^{(q_i, q_j, q_t; r)} = \alpha_R - \sum_{\omega=i,j,t} a_{\omega}^{(q_i, q_j, q_t; r)} \alpha_{\omega} = \frac{N^{(K_i, K_j, K_t, K; \tilde{R})}}{K^2 G(K_i, K_j, K_t, K)}, \quad (4.9)$$

where N has been given in (2.40).

Separating box from pentagon: Having explained how to expand R , now we discuss how to separate box from pentagon in (2.31). First we give an example like $\frac{\langle R \rangle^3}{\langle K \rangle \langle Q_{t_1} \rangle \langle Q_{t_2} \rangle}$ ¹⁰. First using K, K_i, K_j, K_{t_1} to expand one R we will get

$$\frac{\langle R \rangle^3}{\langle K \rangle \langle Q_{t_1} \rangle \langle Q_{t_2} \rangle} \rightarrow \frac{\langle R \rangle^2}{\langle Q_{t_1} \rangle \langle Q_{t_2} \rangle} + \frac{\langle R \rangle^2}{\langle K \rangle \langle Q_{t_2} \rangle}$$

For the first term we expand R using K, K_i, K_j, K_{t_1} while for the second term we expand the R using K, K_i, K_j, K_{t_2} , thus we get

$$\left(\frac{\langle R \rangle}{\langle Q_{t_2} \rangle} + \frac{\langle R \rangle \langle K \rangle}{\langle Q_{t_1} \rangle \langle Q_{t_2} \rangle} \right) + \left(\frac{\langle R \rangle}{\langle Q_{t_2} \rangle} + \frac{\langle R \rangle}{\langle K \rangle} \right)$$

Among these four terms, the last one contributes to the box only. For the first three terms, we expand the remaining R and arrive

$$\left(\left[c_1 + \frac{\langle K \rangle}{\langle Q_{t_2} \rangle} \right] + \left[\frac{\langle K \rangle}{\langle Q_{t_2} \rangle} + \frac{\langle K \rangle^2}{\langle Q_{t_1} \rangle \langle Q_{t_2} \rangle} \right] \right) + \left(\left[c_2 + \frac{\langle K \rangle}{\langle Q_{t_2} \rangle} \right] + \frac{\langle R \rangle}{\langle K \rangle} \right)$$

The last step is to use $Q_i, Q_j, Q_{t_1}, Q_{t_2}$ to expand K for the fourth term

$$\frac{\langle P_1 | K | P_2 \rangle}{\langle P_1 | Q_t | P_2 \rangle \langle P_1 | Q_s | P_2 \rangle} = \frac{-1}{\alpha_K} \left(\frac{\alpha_s}{\langle P_1 | Q_t | P_2 \rangle} + \frac{\alpha_t}{\langle P_1 | Q_s | P_2 \rangle} \right),$$

and we arrive

$$\left(\left[c_1 + \frac{\langle K \rangle}{\langle Q_{t_2} \rangle} \right] + \left[\frac{\langle K \rangle}{\langle Q_{t_2} \rangle} + \left(\frac{\langle K \rangle}{\langle Q_{t_1} \rangle} + \frac{\langle K \rangle}{\langle Q_{t_2} \rangle} \right) \right] \right) + \left(\left[c_2 + \frac{\langle K \rangle}{\langle Q_{t_2} \rangle} \right] + \frac{\langle R \rangle}{\langle K \rangle} \right).$$

Now we have got the complete splitting. The first, the sixth and the eighth terms contribute to the box only. The fourth term contributes to the pentagon (K, K_i, K_j, K_{t_1}) only. The second, the third, the fifth and the seventh terms contribute to the pentagon (K, K_i, K_j, K_{t_2}) only. In our splitting, we have carefully chosen the way to expand R , so that the contribution to the pentagon (K, K_i, K_j, K_{t_1}) appears only once while the contribution to the pentagon (K, K_i, K_j, K_{t_2}) appears four times. However, it can be checked that the sum of these four terms does produce only one term.

¹⁰For simplicity we have used such short notation $\langle R \rangle = \langle P_1 | R | P_2 \rangle$. By comparing with (2.31), we hope its meaning is obvious.

The above splitting can be generalized to arbitrary k and $n \geq -2$. First we define

$$\begin{aligned} B^1[n, k] &= \frac{\langle P_1|R|P_2 \rangle^{n+k}}{\langle P_1|K|P_2 \rangle^{n+2} \prod_{t=1, t \neq i, j}^k \langle P_1|Q_t|P_2 \rangle}, \\ B^2[n, k] &= \{P_{ij,1} \rightarrow P_{ij,2}\}. \end{aligned} \quad (4.10)$$

For the simplest example $k = 3$ we will have (for example, $t = 3, i = 1, j = 2$)

$$B^1[n, 3] = \sum_{s=0}^{n+2} C_s[n, 3] \frac{\langle P_1|R|P_2 \rangle^s}{\langle P_1|K|P_2 \rangle^s} + F[n, 3] \frac{\langle P_1|K|P_2 \rangle}{\langle P_1|Q_3|P_2 \rangle} \quad (4.11)$$

where (4.8) has been used. In the above equation, the first term give the true box coefficient, while the second term, the pentagon coefficient. The expression of $C_s[n, 3]$ and $F[n, 3]$ can be obtained by induction on n as

$$F[n, 3] = \beta^{(q_i, q_j, q_3; r)^{n+3}}, \quad C_s[n, 3] = a_3^{(q_i, q_j, q_3; r)} \beta^{(q_i, q_j, q_3; r)^{n+2-s}}. \quad (4.12)$$

For $k \geq 4$, we use the induction on k and get the complete splitting.

The contribution to the pentagon part has been given in [48] (with a generalization to the massive case) and its evaluation gives (4.1) while the contribution to box part is given by the following sum

$$C[Q_i, Q_j]^{(n, k)} = \sum_{z_1 + \dots + z_k + s = n+2} \left(\prod_{t=1, t \neq i, j}^k a_t^{(q_i, q_j, q_t; r)} \left(\beta^{(q_i, q_j, q_t; r)} \right)^{z_t} \right) \left(\frac{\langle P_1|R|P_2 \rangle^s}{\langle P_1|K|P_2 \rangle^s} + \{P_1 \rightarrow P_2\} \right) \quad (4.13)$$

where $s, z_t \geq 0$ and in the sum $z_1 + \dots + z_k + s = n+2$, z_i, z_j should be excluded. This formula is completely symmetric on t .

4.3 Evaluation of box coefficients

Now we need to evaluate (4.13), where the sum $\left(\frac{\langle P_1|R|P_2 \rangle^s}{\langle P_1|K|P_2 \rangle^s} + \{P_1 \rightarrow P_2\} \right)$ appears. This sum is a special case of the typical sum defined in (A.1) and its final expression is given in (A.11). If we put all $Q_i \rightarrow K$ and $T \rightarrow R$ in (A.11) we will get box coefficients.

However, there is a technical issue related to the u -dependence (i.e., the μ^2 -dependence part, which indicates the dimensional shifted basis) contained inside the definition of R . To have clear separations of u -dependence, we will expand R smartly. To do so, we construct the vector $q_0^{q_i, q_j, K}$ orthogonal to all three momenta K_i, K_j, K

$$(q_0)_\mu^{q_i, q_j, K} = \frac{1}{K^2} \epsilon_{\mu\nu\rho\xi} q_i^\nu q_j^\rho K^\xi = \frac{1}{K^2} \epsilon_{\mu\nu\rho\xi} K_i^\nu K_j^\rho K^\xi. \quad (4.14)$$

Then we can expand R using $Q_i, Q_j, K, (q_0)_\mu^{q_i, q_j, K}$ and obtain

$$\langle P_1|R|P_2 \rangle = \beta \sqrt{1-ua_0^{(q_i, q_j, q_0; r)}} \langle P_1|q_0|P_2 \rangle + \beta^{(q_i, q_j, q_t; r)} \langle P_1|K|P_2 \rangle \quad (4.15)$$

with

$$a_0^{(q_i, q_j, q_0; r)} = \frac{r \cdot q_0^{(q_i, q_j, K)}}{(q_0^{(q_i, q_j, K)})^2} \quad (4.16)$$

$$\beta^{(q_i, q_j, q_0; r)} = \frac{N^{(K_i, K_j, K; \tilde{R})}}{K^2 G(K_i, K_j, K)} \quad (4.17)$$

where N and G are defined in (2.39) and (2.37). The expression (4.15) has the clear u -dependence.

Putting the expansion (4.15) back, we have

$$\frac{\langle P_1 | R | P_2 \rangle^s}{\langle P_1 | K | P_2 \rangle^s} = \sum_{h=0}^s \binom{s}{h} a_0^{(q_i, q_j, q_0; r)^h} \beta^{(q_i, q_j, q_0; r)^{s-h}} \frac{(\beta \sqrt{1-u})^h \langle P_1 | q_0 | P_2 \rangle^h}{\langle P_1 | K | P_2 \rangle^h}. \quad (4.18)$$

Summing the above result with the term coming from exchanging P_1 and P_2 and using the formula (A.11) in the Appendix, we have

$$\begin{aligned} & \frac{(\beta \sqrt{1-u})^h \langle P_1 | q_0 | P_2 \rangle^h}{\langle P_1 | K | P_2 \rangle^h} + \frac{(\beta \sqrt{1-u})^h \langle P_2 | q_0 | P_1 \rangle^h}{\langle P_2 | K | P_1 \rangle^h} \\ &= \begin{cases} \frac{2(2i)^h (q_0^2)^h \{\beta^2(1-u)[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2] + 4K^2[\alpha_i \alpha_j (2q_i \cdot q_j) - \alpha_i^2 q_j^2 - \alpha_j^2 q_i^2]\}^{h/2}}{[(2q_i \cdot q_j)^2 - 4q_i^2 q_j^2]^h}, & \text{for } h \text{ even;} \\ 0, & \text{for } h \text{ odd.} \end{cases} \end{aligned} \quad (4.19)$$

Thus

$$\frac{\langle P_1 | R | P_2 \rangle^s}{\langle P_1 | K | P_2 \rangle^s} + \{P_1 \leftrightarrow P_2\} = \sum_{\text{even } h=0}^s \binom{s}{h} \frac{N^{(K_i, K_j, K; \tilde{R})^{s-h}} 2T}{(K^2 G(K_i, K_j, K))^s}, \quad (4.20)$$

where¹¹

$$\begin{aligned} T(h) &= \left\{ \beta^2(1-u)G(K_i, K_j, K) - K^2 \left[2\alpha_i \alpha_j G \begin{pmatrix} K & K_j \\ K & K_i \end{pmatrix} - \alpha_i^2 G(K, K_j) - \alpha_j^2 G(K, K_i) \right] \right\}^{h/2} \\ &\quad \left(-K^2 G(K_i, K_j, \tilde{R}, K) \right)^{h/2}. \end{aligned} \quad (4.21)$$

Combining Eq.(4.13) and (4.20) the box coefficients are given by

$$\begin{aligned} C[Q_i, Q_j, K] &= \sum_{z_1 + \dots + z_k + s = n+2} \sum_{h=0}^s \left(\prod_{t=1, t \neq i, j}^k \frac{G \begin{pmatrix} K_i & K_j & K_t & K \\ K_i & K_j & \tilde{R} & K \end{pmatrix}}{G(K_i, K_j, K_t, K)} \left(\frac{N^{(K_i, K_j, K_t, K; \tilde{R})}}{G(K_i, K_j, K_t, K)} \right)^{z_t} \right) \\ &\quad \times \binom{s}{h} \frac{N^{(K_i, K_j, K; \tilde{R})^{s-h}} T(h)}{(G(K_i, K_j, K))^s}; \quad \text{with } h \text{ even} \end{aligned} \quad (4.22)$$

¹¹Also $\beta, u, \alpha_i, \alpha_j$ have K^2 in denominators. It can be checked that the overall T does not have K^2 in the denominator. This is important, because the box coefficient (4.22) will not have K^2 as its singularity.

where T is defined in Eq.(4.21). The analysis of the singularity structure of (4.22) has been given in the first subsection.

5. Coefficients of triangle

The triangle coefficient is given in (2.34) and we recall here that when $n \geq -1$,

$$C[Q_i, K] = \frac{(K^2)^{n+1}}{2} \frac{1}{(\sqrt{\Delta})^{n+1}} \frac{1}{(n+1)! \langle P_1 P_2 \rangle^{n+1}} \times \frac{d^{n+1}}{d\tau^{n+1}} \left(\frac{\langle \ell | R Q_i | \ell \rangle^{n+k}}{\prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \Big|_{\ell \rightarrow P_1 - \tau P_2} + \{P_1 \leftrightarrow P_2\} \right) \Big|_{\tau \rightarrow 0} \quad (5.1)$$

where P_1, P_2 are two null momenta constructed from Q_i, K as given in (2.32). More explicitly P_1 and P_2 are given by

$$P_{1,2} = Q_i + x_{1,2} K \quad (5.2)$$

with

$$x_{1,2} = \frac{-2\alpha_i K^2 \pm \sqrt{\Delta}}{2K^2}, \quad \sqrt{\Delta} = \beta \sqrt{1-u} \sqrt{\delta}, \quad \delta = -4q_i^2 K^2. \quad (5.3)$$

To have a good separation of the u -dependence, we can also construct two null momenta $p_{1,2}$ from q_i and K

$$p_{1,2} = q_i + y_{1,2} K, \quad y_{1,2} = \pm \frac{\sqrt{\delta}}{2K^2}. \quad (5.4)$$

Comparing definitions (5.2) with (5.4) we have

$$P_{1,2} = \beta \sqrt{1-u} p_{1,2}, \quad (5.5)$$

thus the triangle coefficient (5.1) [48] can be rewritten as

$$C[Q_i, K] = \frac{(K^2)^{n+1}}{2} \frac{1}{(\sqrt{\delta})^{n+1}} \frac{1}{(n+1)! \langle p_1 p_2 \rangle^{n+1}} \times \frac{d^{n+1}}{d\tau^{n+1}} \left(\frac{\langle \ell | \tilde{r} Q_i | \ell \rangle^{n+k}}{\prod_{t=1, t \neq i}^k \langle \ell | \tilde{q}_t Q_i | \ell \rangle} \Big|_{\ell \rightarrow p_1 - \tau p_2} + \{p_1 \leftrightarrow p_2\} \right) \Big|_{\tau \rightarrow 0}, \quad (5.6)$$

where

$$\tilde{r} = r - \frac{\alpha_R}{\alpha_i} q_i, \quad \tilde{q}_t = q_t - \frac{\alpha_t}{\alpha_i} q_i. \quad (5.7)$$

The good property of expression (5.6) is that only Q_i s have the u -dependence. Now we will evaluate residues based on this expression (5.6).

The presentation of this section is following. In the first subsection we present the result and analyze the singularity structure. For readers who cares only the result, reading this subsection is enough. In subsection 5.2, we will evaluate the derivative part in the expression (5.6) and finally we give the Lorentz-invariant form in subsection 5.3, where the polynomial property of u is a natural by-product.

5.1 The summary of main results of current section

The Lorentz invariant form of external momenta of the triangle coefficient is given by

$$C[Q_i, K] = \frac{(K^2)^{2(n+1)}}{(-2)^{n+1}} \sum_{s=0}^{n+1} \sum_{s'=0}^{\lfloor s/2 \rfloor} \sum_{\substack{\{z_1, z_2, \dots, z_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k z_t = n+1-s}} \frac{(n+k)! T_1(s, s') T_2(z_t)}{s'! (s-2s')! (n+k-s+s')!} \\ \times \left(\prod_{t=1, t \neq i}^k \frac{1}{G(K_i, K_t, K)^{1+z_t}} \right) \left(\sum_{\substack{\{1+z_1, 1+z_2, \dots, 1+z_k\} \\ \{h_1, h_2, \dots, h_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k h_t = \text{even}}} \frac{T_3(z_t, h_t)}{G(K_i, K)^{n+1-h/2}} \right), \quad (5.8)$$

where $h = \sum_{t=1, t \neq i}^k h_t$. Various functions T_1, T_2, T_3 can be found in (5.24) and G is the Gram determinant defined in (2.36) and (2.37).

From (5.8) we can easily read out the analytic structure of triangle coefficients:

- First the coefficient contains only second-type singularities and the first-type singularity related to the triangle topology appears only in the triangle scalar basis (with dimensional shifted basis).
- There are only two kinds of second-type singularities. The first kind of second-type singularities is given by $G(K_i, K) = 0$, which is the second-type singularity intrinsically related to the triangle topology specified by momenta K_i, K . The highest degree of the pole $G(K_i, K)$ is $(n+1)$. It fits with the naive observation in the reduction, i.e., among $(n-k)$ inner momenta $\tilde{\ell}$ in the numerator, $(k-1)$ of them have been used to remove $(k-1)$ propagators, thus it is left with $(n+1) \tilde{\ell}$ in numerator contributing to the triangle topology. Each $\tilde{\ell}$ will bring one factor $G(K_i, K)$ in the denominator of the coefficient, thus we will have the degree $(n+1)$.
- For the pole $G(K_i, K, K_t)$, which is the second-type singularity intrinsically related to the box topology specified by momenta K_i, K_t, K , the highest degree is $(n+2)$. Its appearance is very natural since these boxes can be reduced to triangle by pinching one propagator. In other words, their influence to the triangle is given by the appearance of the factor $G(K_i, K_t, K)$. Moreover, it fits with the naive observation in the reduction and is, in fact, the same highest degree found for the box coefficient in the previous section. The same highest degree $(n+2)$ is also necessary for the cancelation of soft or collinear singularities between box and triangle contributions.

It is worth to mention that when $k=1$, there is no box coefficient at all. From (5.8), we can see that the pole $G(K_i, K, K_t)$ will not appear, which is consistent.

- Similarly to the box case, we need to check the u -dependence part in the numerator. From (5.8), all u -dependence comes from factors T_1, T_2 and its highest degree is $\lfloor (n+1)/2 \rfloor$. It is also important to notice that each u will be accompanied by a factor $G(K_i, K)$ (see Eq.(5.24)), which will reduce the degree of the pole $G(K_i, K)$ for these (rational) parts.

5.2 Evaluation of the derivative part

The (5.6) contains the standard sum defined in (A.1), but there is also the differential action. Thus to apply the result in Appendix, we need to evaluate the derivative part first. Let us define

$$f = \langle \ell | \tilde{r} Q_i | \ell \rangle^{n+k}, \quad g = \frac{1}{\prod_{t=1, t \neq i}^k \langle \ell | \tilde{q}_t Q_i | \ell \rangle}, \quad (5.9)$$

then the derivative gives

$$\frac{d^{n+1}(fg)}{d\tau^{n+1}} = \sum_{s=0}^{n+1} \binom{n+1}{s} f^{(s)} g^{(n+1-s)}, \quad (5.10)$$

where $(*)^{(s)}$ denote the s -th order derivative of the function $(*)$. The Q_i is a linear combination of $p_{1,2}$

$$Q_i = \mu_1 p_1 + \mu_2 p_2, \quad \mu_{1,2} = \frac{\beta \sqrt{1-u}}{2} \pm \frac{\alpha_i}{2y_1} \quad (5.11)$$

The evaluation of $f^{(s)}$: After some algebraic manipulations, we can easily get

$$\langle p_1 - \tau p_2 | \tilde{r} Q_i | p_1 - \tau p_2 \rangle = \langle p_1 | p_2 \rangle a_0 (\tau - \tau_{0,1}) (\tau - \tau_{0,2}) \quad (5.12)$$

where

$$a_0 = \mu_1 \langle p_2 | \tilde{r} | p_1 \rangle, \quad \tau_{0,1} = \frac{\frac{\alpha_i}{y_1} (2\tilde{r} \cdot q_i) + \sqrt{\Omega(\tilde{r})}}{2a_0}, \quad \tau_{0,2} = \frac{\frac{\alpha_i}{y_1} (2\tilde{r} \cdot q_i) - \sqrt{\Omega(\tilde{r})}}{2a_0}. \quad (5.13)$$

and

$$\begin{aligned} \Omega(\tilde{r}) &= (\mu_2 \langle p_2 | \tilde{r} | p_2 \rangle - \mu_1 \langle p_1 | \tilde{r} | p_1 \rangle)^2 + 4\mu_1 \mu_2 \langle p_2 | \tilde{r} | p_1 \rangle \langle p_1 | \tilde{r} | p_2 \rangle \\ &= \frac{\alpha_i^2}{y_1^2} (2\tilde{r} \cdot q_i)^2 + 4 \left(\beta^2 (1-u) - \frac{\alpha_i^2}{y_1^2} \right) ((q_i \cdot \tilde{r})^2 - q_i^2 \tilde{r}^2) \end{aligned} \quad (5.14)$$

with the explicit u -dependence.

To continue, we need the following formula

$$(b_1 b_2 \dots b_n)^{(k)} = \sum_{z_1 + z_2 + \dots + z_n = k} \frac{k!}{z_1! z_2! \dots z_n!} b_1^{(z_1)} b_2^{(z_2)} \dots b_n^{(z_n)}. \quad (5.15)$$

After we set $b_1 = b_2 = \dots = a_0(\tau - \tau_{0,1})(\tau - \tau_{0,2})$, to have nonzero result, $0 \leq z_j \leq 2$. Using s' to denote the number of b_i having the second-order derivative (so there must be $(k - 2s')$ of b_i having the first-order derivative), we have

$$(b_1 b_2 \dots b_n)^{(k)} = \sum_{s'=0}^{[k/2]} \binom{n}{s'} \binom{n-s'}{k-2s'} k! (a_0)^{s'} [a_0(-\tau_{0,1} - \tau_{0,2})]^{k-2s'} [a_0 \tau_{0,1} \tau_{0,2}]^{n-k+s'}, \quad (5.16)$$

where we have take $\tau \rightarrow 0$. Substituting $n \rightarrow n+k, k \rightarrow s$ into the above result, we obtain

$$f^{(s)} = \langle p_1 p_2 \rangle^{n+k} \sum_{s'=0}^{[s/2]} \binom{n+k}{s'} \binom{n+k-s'}{s-2s'} s! \left(- \left(\beta^2(1-u) - \frac{\alpha_i^2}{y_1^2} \right) \frac{(\tilde{r}|\tilde{r})}{K^2} \right)^{s'} \\ \times \left(-\frac{\alpha_i}{y_1} (2\tilde{r} \cdot q_i) \right)^{s-2s'} (-\mu_2 \langle p_1 | \tilde{r} | p_2 \rangle)^{n+k-s} \quad (5.17)$$

where we have used the short notation $(\tilde{r}_1 | \tilde{r}_2) \equiv (\tilde{r}_1 | \tilde{r}_2)_{q_i, K}$ defined in (2.38) since in this section, q_i, K are fixed.

The evaluation of $g^{(n+1-s)}$: Similar to f , g can be written as

$$g = \frac{1}{\langle p_1 p_2 \rangle^{k-1}} \prod_{t=1, t \neq i}^k \frac{1}{a_t(\tau_{t,1} - \tau_{t,2})} \left(\frac{1}{\tau - \tau_{t,1}} - \frac{1}{\tau - \tau_{t,2}} \right) \quad (5.18)$$

where $a_t, \tau_{t,1}$ and $\tau_{t,2}$ are given in (5.13) with \tilde{r} replaced by \tilde{q}_t . Then from Eq.(5.15) we can get

$$g^{(n+1-s)} = \frac{(n+1-s)!}{\langle p_1 p_2 \rangle^{k-1}} \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = n+1-s \\ z_t \geq 0}} \prod_{t=1, t \neq i}^k \frac{1}{z_t! a_t(\tau_{t,1} - \tau_{t,2})} \left(\frac{1}{\tau - \tau_{t,1}} - \frac{1}{\tau - \tau_{t,2}} \right)^{(z_t)} \\ = \frac{(n+1-s)!}{\langle p_1 p_2 \rangle^{k-1}} \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = n+1-s \\ z_t \geq 0}} \prod_{t=1, t \neq i}^k \frac{1}{\sqrt{\Omega(q_t)}} \left(\frac{1}{\tau_{t,2}^{1+z_t}} - \frac{1}{\tau_{t,1}^{1+z_t}} \right), \quad \tau \rightarrow 0. \quad (5.19)$$

Substituting expressions of $\tau_{t,1}$ and $\tau_{t,2}$ yields

$$g^{(n+1-s)} = \frac{(n+1-s)!}{\langle p_1 p_2 \rangle^{k-1}} \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = n+1-s \\ z_t \geq 0}} \prod_{t=1, t \neq i}^k \frac{\sum_{\gamma_t=0}^{[z_t/2]} 2 \binom{1+z_t}{2\gamma_t+1} (\Omega(\tilde{q}_t))^{\gamma_t} \left(\frac{\alpha_i}{y_1} (2\tilde{q}_t \cdot q_i) \right)^{z_t-2\gamma_t}}{(-2\mu_2 \langle p_1 | \tilde{q}_t | p_2 \rangle)^{1+z_t}} \quad (5.20)$$

The final result of derivation: Putting all together and performing a bit algebraic manipulations, we can write Eq.(5.6) as

$$C[Q_i, K] = \frac{(K^2)^{n+1}}{2} \frac{1}{(-2q_i^2)^{n+1}} \sum_{s=0}^{n+1} \sum_{s'=0}^{[s/2]} \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = n+1-s \\ z_t \geq 0}} \frac{(n+k)!}{s'!(s-2s')!(n+k-s+s')!} \\ \times T_1(s, s') T_2(z_t) \left(\frac{\langle p_1 | \tilde{r} | p_2 \rangle^{n+k-s}}{\prod_{t=1, t \neq i}^k \langle p_1 | \tilde{q}_t | p_2 \rangle^{1+z_t}} + \{p_1 \leftrightarrow p_2\} \right), \quad (5.21)$$

where the Lorentz invariant forms of T_1, T_2 are

$$T_1(s, s') = \left((\alpha_i^2 - y_1^2 \beta^2 (1 - u)) \frac{(\tilde{r}|\tilde{r})}{K^2} \right)^{s'} (-\alpha_i (2\tilde{r} \cdot q_i))^{s-2s'},$$

$$T_2(z_t) = \prod_{t=1, t \neq i}^k \sum_{\gamma_t=0}^{[z_t/2]} \binom{1+z_t}{2\gamma_t+1} \left(\frac{1}{4} y_1^2 \Omega(\tilde{q}_t) \right)^{\gamma_t} (\alpha_i (\tilde{q}_t \cdot q_i))^{z_t-2\gamma_t}. \quad (5.22)$$

The u -dependence is entirely in T_1 and T_2 , thus the polynomial property of u is obvious.

5.3 The Lorentz-invariant Form

In (5.21), the sum inside the bracket is the standard one defined in Appendix (A.1). Thus we can use the result (A.11) given in the Appendix. First noticing that $\langle p_1 | q_i | p_2 \rangle = 0$ and $\langle p_2 | q_i | p_1 \rangle = 0$ by our construction (5.4), $\langle p_1 | \tilde{q}_t | p_2 \rangle = \langle p_1 | q_t | p_2 \rangle$ and $\langle p_1 | \tilde{r} | p_2 \rangle = \langle p_1 | r | p_2 \rangle$ in (5.21). After some algebraic calculations, Eq.(5.21) leads to

$$C[Q_i, K] = \frac{(K^2)^{2(n+1)}}{(-2)^{n+1}} \sum_{s=0}^{n+1} \sum_{s'=0}^{[s/2]} \sum_{\substack{\{z_1, z_2, \dots, z_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k z_t = n+1-s}} \frac{(n+k)! T_1(s, s') T_2(z_t)}{s'! (s-2s')! (n+k-s+s')!}$$

$$\times \left(\prod_{t=1, t \neq i}^k \frac{1}{G(K_i, K_t, K)^{1+z_t}} \right) \left(\sum_{\substack{\{1+z_1, 1+z_2, \dots, 1+z_k\} \\ \{h_1, h_2, \dots, h_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k h_t = \text{even}}} \frac{T_3(z_t, h_t)}{G(K_i, K)^{n+1-h/2}} \right), \quad (5.23)$$

where $h = \sum_{t=1, t \neq i}^k h_t$, G is Gram determinant defined in (2.36) and (2.37) and

$$T_1(s, s') = \left(\Omega_1(\tilde{R}) \right)^{s'} \left(2\Omega_2(\tilde{R}) \right)^{s-2s'},$$

$$T_2(z_t) = \prod_{t=1, t \neq i}^k \sum_{\gamma_t=0}^{[z_t/2]} \binom{1+z_t}{2\gamma_t+1} \left(\Omega_1(K_t) + (\Omega_2(K_t))^2 \right)^{\gamma_t} (-\Omega_2(K_t))^{z_t-2\gamma_t},$$

$$T_3(z_t, h_t) = \prod_{t=1, t \neq i}^k \binom{1+z_t}{h_t} \left(\epsilon(\tilde{R}, K_i, K_t, K) \right)^{h_t} \left(G \begin{pmatrix} K_i & K & K_t \\ K_i & K & \tilde{R} \end{pmatrix} \right)^{1+z_t-h_t}, \quad (5.24)$$

with

$$\Omega_1(\tilde{R}) = \left(\alpha_i^2 + \frac{G(K_i, K)}{(K^2)^2} \beta^2 (1 - u) \right) \frac{G(K_i, \tilde{R}, K)}{K^2},$$

$$\Omega_2(\tilde{R}) = \frac{1}{K^2} \left(\alpha_R G(K, K_i) - \alpha_i G \begin{pmatrix} K & K_i \\ K & \tilde{R} \end{pmatrix} \right). \quad (5.25)$$

It is worth to mention that it can be checked that Ω_1 has $(K^2)^4$ in the denominator and Ω_2 has $(K^2)^2$ in the denominator. When putting back into (5.23), the K^2 factor from Ω_1, Ω_2 will be canceled by the overall $(K^2)^{2(n+1)}$ factor. In other words, K^2 will not be a singularity for the triangle coefficient.

Since our main concern is the highest degrees of poles $G(K_i, K)$ and $G(K_i, K_t, K)$, we will discuss how to get this information from (5.23). For the pole $G(K_i, K_t, K)$ there is one and only one term with highest degree in the expression (5.23) which is given by $s = 0, s' = 0, z_t = n - 1$ and $z_r = 0$ for $r \neq i, t$. In other words, the highest degree of the pole $G(K_i, K_t, K)$ is $(n + 2)$.

For the pole $G(K_i, K)$, since there are many terms contributing to the highest degree in the expression (5.23), it will be a little more complicated and we will use another expression to discuss. Since $G(K_i, K) = K^2 q_i^2$, we will rewrite (5.23) using q_i^2 . Noting that

$$T_1(s, s') = 2^{s-2s'} (-\alpha_i(r \cdot q_i))^s,$$

$$T_2(z_t) = \prod_{t=1, t \neq i}^k (1 + z_t)(\alpha_i(q_t \cdot q_i))^{z_t}.$$

therefore, after removing terms with q_i^2 in the numerator, we have

$$C[Q_i, K] \rightarrow \frac{(K^2)^{2(n+1)} \alpha_i^{n+1} (-r \cdot q_i)^{n+k}}{(-2)^{n+1} (q_i^2)^{n+1}} \sum_{s=0}^{n+1} \sum_{s'=0}^{[s/2]} \frac{(n+k)! 2^{s-2s'}}{s'! (s-2s')! (n+k-s+s')!}$$

$$\times \sum_{\substack{\{z_1, z_2, \dots, z_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k z_t = n+1-s}} \left(\prod_{t=1, t \neq i}^k \left(\frac{(1+z_t)(q_t \cdot q_i)^{1+2z_t}}{(q_i^2 q_t^2 - (q_i \cdot q_t)^2)^{1+z_t}} \right) \right) \quad (5.26)$$

With this explicit form, the highest degree of the pole q_i^2 (or the pole $G(K_i, K)$) is $(n + 1)$.

6. Coefficients of bubble

After accomplishing the triangle coefficients, the last thing is to derive the coefficient of the bubble. The bubble coefficient is the sum of the residues of the poles from the following expression

$$B = \sum_{i=1}^k \sum_{q=0}^n \frac{-(K^2)^{n+1} \langle \ell | R Q_i | \ell \rangle^{n-q+k-1}}{\langle \ell | K Q_i | \ell \rangle^{n-q+1} \prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \frac{1}{q+1} \frac{\langle \ell | R | \ell \rangle^{q+1}}{\langle \ell | K | \ell \rangle^{q+1}}. \quad (6.1)$$

This expression is for $k \geq 1$. For $k = 0$, the answer is very simple and we write down here¹²

$$C[K]_{k=0} = \frac{\sum_{z=0}^{[(n+1)/2]} (-2\alpha_R K^2)^{n-2z} (-4\beta^2(1-u)G(K, \tilde{R}))^z}{2^{n+1}(n+1)} \quad (6.2)$$

¹²With the definition of (2.26) and (2.17), we can see the overall $(K^2)^{-n}$ -dependence, which is the only singularity for the case $k = 0$.

As in previous two sections, we summarize the final result and discuss the analytic property in the first subsection. The derivation of the result is given in the next three subsections. In subsection 6.2, we present the explicit spinor form after the evaluations of residues. In subsection 6.3, we deal with the derivative part and finally in subsection 6.4, we translate the spinor form into the Lorentz-invariant form.

6.1 The summary of main result of current section

The Lorentz invariant form of bubble coefficient is given by

$$\begin{aligned}
C[K] = & \sum_{i=1}^k \sum_{q=0}^n (-1)^{n-q} (K^2)^{2n+1-q} \sum_{s=\text{Max}\{n-2q-1,0\}}^{n-q} \sum_{s_1=0}^s \sum_{s'_1=0}^{[s_1/2]} T_0(s, s_1, s'_1) T_1(s_1, s'_1) \\
& \left(-\frac{G(K_i, \tilde{R}, K)}{K^2} \right)^{n-q-s} \times \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = s-s_1 \\ z_t \geq 0}} \sum_{r_1=0}^{2q+1+s-n} \sum_{r_2=0}^{n-q-s} \frac{T_2(z_t) T_4(r_1, r_2)}{(-4G(K_i, K))^{(n-q-s+1+r_1-r_2)/2}} \\
& \times \left(2 \prod_{t=1, t \neq i}^k \frac{1}{G(K_i, K_t, K)^{1+z_t}} \right) \left(\sum_{\substack{\{1+z_1, 1+z_2, \dots, 1+z_k\} \\ \{h_1, h_2, \dots, h_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k h_t = \text{even}}} \frac{T_3(z_t, h_t)}{G(K_i, K)^{n-q-h/2}} \right) \quad (6.3)
\end{aligned}$$

where T_0, T_4 can be found in (6.26) and T_1, T_2, T_3 are defined in Eq.(5.22). In the sum (6.3), we need to have $(n - q - s + 1 + r_1 - r_2)$ and $h = \sum_{t=1, t \neq i}^k h_t$ to be even number.

From (6.3), the analytic property of bubble coefficients can be read out as follows¹³:

- Like coefficients of the box and triangle, only second-type singularities appear in bubble coefficients (remembering the first-type singularity of the bubble is $(K^2 - (M_1 \pm M_2)^2)$). There are three second-type singularities: $G(K, K_i, K_j)$ related to the box topology, $G(K, K_i)$ related to the triangle topology and K^2 related to the bubble topology.
- The highest degree of the pole K^2 is n . K^2 is the intrinsic second-type singularity related to the bubble topology. Its highest degree fits the naive observation in the reduction: to remove k propagators from the denominator we need to reduce the k 's $\tilde{\ell}$ in the numerator.
- The highest degree of the pole $G(K, K_i)$ is $(n + 1)$, which fits with the naive observation in the reduction. It is also the same as the pole $G(K, K_i)$ appearing in triangle coefficients. Having the same highest degree is reasonable when we consider some soft or collinear limits of full one-loop amplitudes after combining all contributions (such as box, triangle and bubble) together.
- The highest degree of the pole $G(K, K_i, K_j)$ is $(n + 1)$. It is worth to recall that the highest degree of the same pole in box and triangle coefficients is $(n + 2)$. This is because to get the influence of the box to the bubble, one further reduction from the triangle to the bubble is needed.

¹³The derivation of the highest degree can be found in subsection 6.4.

- To see the dimensional shifted basis (which is related to rational part of one-loop amplitudes (2.4)), we need to check the u -dependence part in the numerator. The highest degree of u is $[n/2]$.

6.2 Spinor form of the bubble coefficient

The expression (6.1) is not yet the spinor form of the coefficient of the bubble. We need to evaluate residues of various poles from $\langle \ell | K Q_i | \ell \rangle$ and $\langle \ell | Q_j Q_i | \ell \rangle$. Among these two kinds of poles, the contributions of poles from $\langle \ell | Q_j Q_i | \ell \rangle$ are zero. To see it, let us start with the typical term

$$B_{i,q} \equiv \frac{-(K^2)^{n+1} \langle \ell | R Q_i | \ell \rangle^{n-q+k-1}}{\langle \ell | K Q_i | \ell \rangle^{n-q+1} \prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \frac{1}{q+1} \frac{\langle \ell | R | \ell \rangle^{q+1}}{\langle \ell | K | \ell \rangle^{q+1}}. \quad (6.4)$$

and construct two massless momenta as (see (2.33))

$$P_{1,2}^{(i,j)} = Q_j + y_{1,2}^{(i,j)} Q_i, \quad (i < j) \quad (6.5)$$

where

$$y_{1,2}^{(i,j)} = \frac{-2Q_i \cdot Q_j \pm \sqrt{\Delta^{(i,j)}}}{2Q_i^2}, \quad \Delta^{(i,j)} = (2Q_i \cdot Q_j)^2 - 4Q_i^2 Q_j^2. \quad (6.6)$$

Then the residues of the poles $P_{1,2}^{(i,j)}$ are

$$\text{Res}(B_{i,q})|_{P_{1,2}^{(i,j)}} = \pm \frac{1}{\sqrt{\Delta^{(i,j)}}} \frac{(K^2)^{n+1} \left\langle P_{1,2}^{(i,j)} | R | P_{2,1}^{(i,j)} \right\rangle^{n-q+k-1}}{\left\langle P_{1,2}^{(i,j)} | K | P_{2,1}^{(i,j)} \right\rangle^{n-q+1} \prod_{t=1, t \neq i,j}^k \left\langle P_{1,2}^{(i,j)} | Q_t | P_{2,1}^{(i,j)} \right\rangle} \frac{1}{q+1} \frac{\left\langle P_{1,2}^{(i,j)} | R | P_{1,2}^{(i,j)} \right\rangle^{q+1}}{\left\langle P_{1,2}^{(i,j)} | K | P_{1,2}^{(i,j)} \right\rangle^{q+1}}$$

where (+)-sign is for the pole $P_1^{(i,j)}$ and (-)-sign, for the pole $P_2^{(i,j)}$. It is worth to notice that the factor $\langle \ell | Q_j Q_i | \ell \rangle$ appears in both $B_{i,q}$ and $B_{j,q}$ up to a minus sign, thus $\text{Res}(B_{i,q})|_{P_{1,2}^{(i,j)}} = -\text{Res}(B_{j,q})|_{P_{1,2}^{(i,j)}}$. So when we sum up all residues, contributions from $\langle \ell | Q_j Q_i | \ell \rangle$ cancel.

Now we consider poles from $\langle \ell | K Q_i | \ell \rangle$, which has been carefully discussed in Eq.(5.2). The residue of P_1 is given by

$$\text{Res}(B_{i,q})|_{P_1} = \frac{(-1)^{n-q} (K^2)^{2n+2-q} (x_1 - x_2)^{n-q+1}}{\langle P_1 P_2 \rangle^{n-q} \Delta^{n-q+1} (q+1)(n-q)!} \frac{d^{n-q}}{d\tau^{n-q}} \left(\frac{\langle \ell | R Q_i | \ell \rangle^{n-q+k-1}}{\prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \frac{\langle \ell | R | P_1 \rangle^{q+1}}{\langle \ell | K | P_1 \rangle^{q+1}} \right) \Big|_{\ell \rightarrow P_1 - \tau P_2},$$

and the residue of P_2

$$\text{Res}(B_{i,q})|_{P_2} = \frac{(-1)^{n-q+1} (K^2)^{2n+2-q} (x_1 - x_2)^{n-q+1}}{\langle P_1 P_2 \rangle^{n-q} \Delta^{n-q+1} (q+1)(n-q)!} \frac{d^{n-q}}{d\tau^{n-q}} \left(\frac{\langle \ell | R Q_i | \ell \rangle^{n-q+k-1}}{\prod_{t=1, t \neq i}^k \langle \ell | Q_t Q_i | \ell \rangle} \frac{\langle \ell | R | P_2 \rangle^{q+1}}{\langle \ell | K | P_2 \rangle^{q+1}} \right) \Big|_{\ell \rightarrow P_2 - \tau P_1}.$$

Using the relation (5.5) and the corresponding $p_{1,2}$ in Eq.(5.4), similarly to the case of the triangle, the above two equations can be simplified as:

$$\begin{aligned} \text{Res}(B_{i,q})|_{P_1} &= \frac{(-1)^{n-q} (K^2)^{n+1}}{\beta(\sqrt{1-u}) \langle p_1 p_2 \rangle^{n-q} \sqrt{\delta}^{n-q+1} (q+1)(n-q)!} \\ &\quad \times \frac{d^{n-q}}{d\tau^{n-q}} \left(\frac{\langle \ell | \tilde{r} Q_i | \ell \rangle^{n-q+k-1}}{\prod_{t=1, t \neq i}^k \langle \ell | \tilde{q} Q_i | \ell \rangle} \frac{\langle \ell | \beta(\sqrt{1-u}) r + \alpha_R K | p_1 \rangle^{q+1}}{\langle \ell | K | p_1 \rangle^{q+1}} \right) \Big|_{\ell \rightarrow p_1 - \tau p_2}, \end{aligned} \quad (6.7)$$

and,

$$\begin{aligned} \text{Res}(B_{i,q})|_{P_2} &= \frac{(-1)^{n-q+1}(K^2)^{n+1}}{\beta(\sqrt{1-u}) \langle p_1 p_2 \rangle^{n-q} \sqrt{\delta}^{n-q+1} (q+1)(n-q)!} \\ &\times \frac{d^{n-q}}{d\tau^{n-q}} \left(\frac{\langle \ell | \tilde{r} Q_i | \ell \rangle^{n-q+k-1}}{\prod_{t=1, t \neq i}^k \langle \ell | \tilde{q}_t Q_i | \ell \rangle} \frac{\langle \ell | \beta(\sqrt{1-u})r + \alpha_R K | p_2 \rangle^{q+1}}{\langle \ell | K | p_2 \rangle^{q+1}} \right) \Big|_{\ell \rightarrow p_2 - \tau p_1}. \end{aligned} \quad (6.8)$$

Summing all together we have the coefficient of the bubble in the spinor form

$$C[K] = \sum_{i=1}^k \sum_{q=0}^n (\text{Res}(B_{i,q})|_{P_1} + \text{Res}(B_{i,q})|_{P_2}). \quad (6.9)$$

6.3 Evaluation of the derivative part

The spinor form (6.9) is complicated and we need to evaluate the derivation first. To do so, we define

$$f \equiv \langle \ell | \tilde{r} Q_i | \ell \rangle^{n-q+k-1}, \quad g \equiv \frac{1}{\prod_{t=1, t \neq i}^k \langle \ell | \tilde{q}_t Q_i | \ell \rangle}, \quad w \equiv \frac{\langle \ell | \beta(\sqrt{1-u})r + \alpha_R K | \ell \rangle^{q+1}}{\langle \ell | K | \ell \rangle^{q+1}}. \quad (6.10)$$

and the derivative is given by

$$\frac{d^{n-q}}{d\tau^{n-q}}(fgw) = \sum_{s=0}^{n-q} \sum_{s_1=0}^s \binom{n-q}{s} \binom{s}{s_1} f^{(s_1)} g^{(s-s_1)} w^{(n-q-s)} \quad (6.11)$$

The evaluation of $f^{(s_1)}$ and $g^{(s-s_1)}$: To get $f^{(s_1)}$ and $g^{(s-s_1)}$, we can use the result in Subsection 4.2. If substituting $s_1, n-q+k-1$ for $s, n+k$ in Eq. (5.17) we get ($\mu_{1,2}$ is given in (5.11))

$$\begin{aligned} f_{P_1}^{(s_1)} &= \langle p_1 p_2 \rangle^{n-q+k-1} \sum_{s'_1=0}^{[s_1/2]} \binom{n-q+k-1}{s'_1} \binom{n-q+k-1-s'_1}{s_1-2s'_1} s_1! \\ &\times \left(-\frac{1}{y_1} \right)^{s_1} T_1(s_1, s'_1) (-\mu_2 \langle p_1 | \tilde{r} | p_2 \rangle)^{n-q+k-1-s_1}, \\ f_{P_2}^{(s_1)} &= (-1)^{s_1} f_{P_1}^{(s_1)} \Big|_{\mu_1 \leftrightarrow \mu_2, p_1 \leftrightarrow p_2}. \end{aligned} \quad (6.12)$$

If substituting $s-s_1$ for $n+1-s$ in Eq. (5.20) we get

$$\begin{aligned} g_{P_1}^{(s-s_1)} &= \frac{(s-s_1)!}{\langle p_1 p_2 \rangle^{k-1}} \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = s-s_1 \\ 0 \leq z_t \leq s-s_1}} \frac{T_2(z_t)}{y_1^{s-s_1} \prod_{t=1, t \neq i}^k (-\mu_2 \langle p_1 | \tilde{q}_t | p_2 \rangle)^{1+z_t}}, \\ g_{P_2}^{(s-s_1)} &= (-1)^{s_1-s} g_{P_1}^{(s-s_1)} \Big|_{\mu_1 \leftrightarrow \mu_2, p_1 \leftrightarrow p_2}, \end{aligned} \quad (6.13)$$

where $T_1(s_1, s'_1)$ and $T_2(z_t)$ are defined by Eq.(5.22) and Eq.(5.24).

The evaluation of $w^{(n-q-s)}$: For $\text{Res}B_{i,q}|_{P_1}$, w is

$$w_{P_1} = \frac{1}{(\sqrt{\delta})^{q+1}} (\beta(\sqrt{1-u})2r \cdot q_i - \tau\beta(\sqrt{1-u}) \langle p_2|r|p_1 \rangle + \alpha_R\sqrt{\delta})^{q+1}. \quad (6.14)$$

So when $s \geq \text{Max}\{n-2q-1, 0\}$

$$\begin{aligned} w_{P_1}^{(n-q-s)} &= \frac{(q+1)!}{(2q+1+s-n)!} \frac{(-\beta\sqrt{1-u})^{n-q-s}}{(\sqrt{\delta})^{q+1}} \\ &\quad \times (\beta(\sqrt{1-u})2r \cdot q_i - \tau\beta(\sqrt{1-u}) \langle p_2|r|p_1 \rangle + \alpha_R\sqrt{\delta})^{2q+1+s-n} \langle p_2|r|p_1 \rangle^{n-q-s}, \end{aligned} \quad (6.15)$$

and when $s < \text{Max}\{n-2q-1, 0\}$, $w_{P_1}^{(n-q-s)} = 0$. After setting $\tau \rightarrow 0$, Eq. (6.15) becomes

$$\begin{aligned} w_{P_1}^{(n-q-s)} &= \frac{(q+1)!}{(2q+1+s-n)!} \frac{(-\beta\sqrt{1-u})^{n-q-s}}{(\sqrt{\delta})^{q+1}} \\ &\quad \times (\beta(\sqrt{1-u})2r \cdot q_i + \alpha_R\sqrt{\delta})^{2q+1+s-n} \langle p_2|r|p_1 \rangle^{n-q-s}, \end{aligned} \quad (6.16)$$

Similarly for $\text{Res}B_{i,q}|_{P_2}$, we have

$$\begin{aligned} w_{P_2}^{(n-q-s)} &= \frac{(q+1)!}{(2q+1+s-n)!} \frac{(-\beta\sqrt{1-u})^{n-q-s}}{(-\sqrt{\delta})^{q+1}} \\ &\quad \times (\beta(\sqrt{1-u})2r \cdot q_i - \alpha_R\sqrt{\delta})^{2q+1+s-n} \langle p_1|r|p_2 \rangle^{n-q-s}. \end{aligned} \quad (6.17)$$

The final result: Now we want to sum up residues of P_1, P_2 of $B_{i,q}$. Up to a common factor, their sum is given by

$$\begin{aligned} &(\beta(\sqrt{1-u})2r \cdot q_i + \alpha_R\sqrt{\delta})^{2q+1+s-n} \mu_2^{n-q-s} \frac{\langle p_1|\tilde{r}|p_2 \rangle^{s+k-1-s_1}}{\prod_{t=1, t \neq i}^k (\langle p_1|\tilde{q}_t|p_2 \rangle)^{1+z_t}} \\ &+ (-1)^{n+s} (\beta(\sqrt{1-u})2r \cdot q_i - \alpha_R\sqrt{\delta})^{2q+1+s-n} \mu_1^{n-q-s} \frac{\langle p_2|\tilde{r}|p_1 \rangle^{s+k-1-s_1}}{\prod_{t=1, t \neq i}^k (\langle p_2|\tilde{q}_t|p_1 \rangle)^{1+z_t}}. \end{aligned} \quad (6.18)$$

Using the binomial expansion

$$(\beta(\sqrt{1-u})2r \cdot q_i + \alpha_R\sqrt{\delta})^{2q+1+s-n} \left(\frac{\beta(\sqrt{1-u})}{2} - \frac{\alpha_i}{2y_1} \right)^{n-q-s} = \sum_{r_1=0}^{2q+1+s-n} \sum_{r_2=0}^{n-q-s} C_{r_1, r_2}(P_1) \quad (6.19)$$

where

$$\begin{aligned} C_{r_1, r_2}(P_1) &= \binom{2q+1+s-n}{r_1} \binom{n-q-s}{r_2} (\beta(\sqrt{1-u})2r \cdot q_i)^{r_1} (\alpha_R\sqrt{\delta})^{2q+1+s-n-r_1} \\ &\quad \times \left(\frac{\beta(\sqrt{1-u})}{2} \right)^{r_2} \left(-\frac{\alpha_i}{2y_1} \right)^{n-q-s-r_2} \end{aligned} \quad (6.20)$$

and similar expression for

$$C_{r_1, r_2}(P_2) = (-1)^{n-q-s-1+r_1+r_2} C_{r_1, r_2}(P_1), \quad (6.21)$$

Eq.(6.18) becomes

$$\sum_{r_1=0}^{2q+1+s-n} \sum_{r_2=0}^{n-q-s} C_{r_1, r_2}(p_1) \left(\frac{\langle p_1 | \tilde{r} | p_2 \rangle^{s+k-1-s_1}}{\prod_{t=1, t \neq i}^k (\langle p_1 | \tilde{q}_t | p_2 \rangle)^{1+z_t}} + \frac{(-1)^{n-q-s-1+r_1+r_2} \langle p_2 | \tilde{r} | p_1 \rangle^{s+k-1-s_1}}{\prod_{t=1, t \neq i}^k (\langle p_2 | \tilde{q}_t | p_1 \rangle)^{1+z_t}} \right). \quad (6.22)$$

Since the bubble coefficient is the polynomial of u , from the factor $(\beta\sqrt{1-u})^{n-q-s-1+r_1+r_2}$ in the sum, only the terms with $(n-q-s-1+r_1+r_2)$ being even numbers are left. In other words, the above expression can be written as

$$\sum_{r_1=0}^{2q+1+s-n} \sum_{r_2=0}^{n-q-s} C_{r_1, r_2}(p_1) \left(\frac{\langle p_1 | \tilde{r} | p_2 \rangle^{s+k-1-s_1}}{\prod_{t=1, t \neq i}^k (\langle p_1 | \tilde{q}_t | p_2 \rangle)^{1+z_t}} + \frac{\langle p_2 | \tilde{r} | p_1 \rangle^{s+k-1-s_1}}{\prod_{t=1, t \neq i}^k (\langle p_2 | \tilde{q}_t | p_1 \rangle)^{1+z_t}} \right). \quad (6.23)$$

for which we can apply the general expression in Appendix (A.1) and (A.11).

6.4 The Lorentz invariant form

Putting all together, the coefficient of the bubble is given by

$$\begin{aligned} C[K] &= \sum_{i=1}^k \sum_{q=0}^n (-1)^{n-q} (K^2)^{2n+1-q} \sum_{s=Max\{n-2q-1, 0\}}^{n-q} \sum_{s_1=0}^s \sum_{s'_1=0}^{[s_1/2]} T_0(s, s_1, s'_1) T_1(s_1, s'_1) \\ &\quad \left(-\frac{G(K_i, \tilde{R}, K)}{K^2} \right)^{n-q-s} \times \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = s-s_1 \\ z_t \geq 0}} \sum_{r_1=0}^{2q+1+s-n} \sum_{r_2=0}^{n-q-s} \frac{T_2(z_t) T_4(r_1, r_2)}{(-4G(K_i, K))^{(n-q-s+1+r_1-r_2)/2}} \\ &\quad \times \left(2 \prod_{t=1, t \neq i}^k \frac{1}{G(K_i, K_t, K)^{1+z_t}} \right) \left(\sum_{\substack{\{1+z_1, 1+z_2, \dots, 1+z_k\} \\ \{h_1, h_2, \dots, h_k\} \geq 0 \\ \sum_{t=1, t \neq i}^k h_t = \text{even}}} \frac{T_3(z_t, h_t)}{G(K_i, K)^{n-q-h/2}} \right), \end{aligned} \quad (6.24)$$

where

$$T_0(s, s_1, s'_1) = \frac{2^s q! (n-q+k-1)!}{(2q+1+s-n)! s'_1! (s_1-2s'_1)! (n-q+k-1-s_1+s'_1)! (n-q-s)!} \quad (6.25)$$

$$\begin{aligned} T_4(r_1, r_2) &= \binom{2q+1+s-n}{r_1} \binom{n-q-s}{r_2} \left(\frac{2}{K^2} G \left(\begin{matrix} K & K_i \\ K & \tilde{R} \end{matrix} \right) \right)^{r_1} \left(\frac{1}{2K^2} \right)^{r_2} \\ &\quad \times (\beta^2(1-u))^{\frac{1}{2}(n-q-s-1+r_1+r_2)} \alpha_R^{2q+1+s-n-r_1} (-\alpha_i)^{n-q-s-r_2} \end{aligned} \quad (6.26)$$

and T_1, T_2, T_3 are defined in Eq.(5.22). In the sum (6.24), we need to have $(n-q-s+1+r_1-r_2)$ and $h = \sum_{t=1, t \neq i}^k h_t$ to be even number.

From (6.24) we can see various second-type singularities. Now we discuss their highest degree. For the pole $G(K_i, K_t, K)$, there is only one term to contribute. By setting $s = n-q$, $q = 0$, $s_1 = 0$, $r_1 = 0$, $1, r_2 = 0$

we find the highest degree is $(n + 1)$. It is different from the highest degree $(n + 2)$ of the same pole in coefficients of the box and triangle.

For the highest degree of the pole K^2 , which is the intrinsic second-type singularity related to bubble topology, we can find

$$C[K] \rightarrow \frac{1}{(K^2)^n} \quad (6.27)$$

by noticing

$$\begin{aligned} T_1 &\rightarrow \frac{1}{(K^2)^{2s_1}} & T_2 &\rightarrow \frac{1}{(K^2)^{2z_t}} \\ T_4 &\rightarrow \frac{1}{(K^2)^{r_1+r_2+(n-q-s-1+r_1+r_2)+2(2q+1+s-n-r_1+n-q-s-r_2)}} \end{aligned}$$

For the pole $G(K_i, K) = K^2 q_i^2$, its highest degree shows up in many terms, so we need to rewrite the result to see clearly. Using $\delta = -4q_i^2 K^2$ and removing all q_i^2 terms in the numerator we find

$$\begin{aligned} C[K] &\rightarrow \frac{(-2)^{n+1}(K^2)^n}{\delta^{n+1}} \alpha_i^n \sum_{s=\text{Max}\{n-1,0\}}^n \sum_{s_1=0}^s \sum_{s'_1=0}^{[s_1/2]} 2^{s_1-2s'_1} T_0(s, s_1, s'_1) (-r \cdot q_i)^{k+s} \\ &\quad \sum_{\substack{\sum_{t=1, t \neq i}^k z_t = s-s_1 \\ 0 \leq z_t \leq s-s_1}} \left(\prod_{t=1, t \neq i}^k \left(\frac{(1+z_t)(q_t \cdot q_i)^{1+2z_t}}{(q_i^2 q_t^2 - (q_i \cdot q_t)^2)^{1+z_t}} \right) \right) \end{aligned}$$

From this expression, we can find the highest degree of pole $G(K_i, K) = K^2 q_i^2$ is $(n + 1)$.

7. Conclusion

In this paper, to prepare the study of analytic properties of one-loop amplitudes, we have rewritten the spinor forms of one-loop coefficients given in [34] to manifestly Lorentz-invariant contraction forms of external momenta. Although the rewriting is a little bit complicated and some skills within the spinor formalism are needed, the final results of various coefficients are manageable and have been summarized in the first subsection of section 4,5,6.

The main results of our calculations are following. Firstly we have found that although there are two types of singularities by the general S-matrix analysis, coefficients of each basis contain only *second-type* singularities. Secondly, the degree of each second-type singularities is tightly related to the degree of the inner momentum in numerators. In other words, when we study the analytic property, not only the structure of the denominator, but also the structure of the numerator, play an important role. For the renormalizable theory, there is an up-bound for the degree of $\tilde{\ell}$ in the numerator, thus the possible highest degree for each second-type singularity is known. For the non-renormalizable theory, the information of the degree of $\tilde{\ell}$ in numerator will also tell us how bad the contributions from these singularities could be.

Thirdly, for a given basis, its coefficient contains not only the second-type singularity related to its topology, but also those related to its mother topology. Not only that, the degree also matches up. For example, the triangle coefficient contains the second-type singularity of the box topology with the same highest degree $(n + 2)$ as the box coefficient. This matching has the physically meaningful cancelation in various singular limits. To have a clear picture, we have given a table (see Table 1) where for each coefficient, the involved singularities and their highest degrees have been given.

Table 1: The table of singularities and their highest degrees for each coefficient

	$D^{(K_i, K_j, K_t, K_\omega, K)}$	$G(K_i, K_j, K_t, K)$	$G(K_i, K_j, K)$	$G(K_i, K)$	K^2
Pentagon	1	$(n + k)$			
Box		$(n + 3)$	$(n + 2)$		
Triangle			$(n + 2)$	$(n + 1)$	
Bubble			$(n + 1)$	$(n + 1)$	n

From the table, there is one point we want to mention. The pole $G(K_i, K_j, K_t, K)$ related to the pentagon topology shows up only in the coefficients of the pentagon and box, while the pole $G(K_i, K_j, K)$ related to the box topology shows up also in the coefficients of the box, triangle and bubble. We believe the reason is that in the $(4 - 2\epsilon)$ -dimension, the pentagon can be expressed as the linear combination of boxes plus terms in the higher order of ϵ . Thus the influence of pentagon can not be propagated to lower topologies. It is consistent with the well known fact that second-type singularity depends on the dimension of space-time and structures of interactions, such as the spins, derivative interactions etc.

We want to emphasize following points for our work. Firstly our paper is to set up a frame for the theoretical study of analytic property of one-loop amplitudes. Thus although it will be possible to use these explicit Lorentz-invariant forms of coefficients in real one-loop calculations numerically or analytically, we will not do it here and leave it as a future project. To use our result in real calculations, we need to discuss the efficiency or stability of calculations as carefully discussed, for example, in paper [53].

One possible application of our results is following. Since our results are complete, i.e., there are $(\mu^2)^n$ -terms corresponding to rational part as mentioned in section 2, we could use our result to calculate the rational terms and compare with results from the recursion relation given in [37, 38, 39]. We believe this calculation will help to us to clarify some points in the recursion relation.

Secondly, our current focus is coefficients of various basis, not the whole structure of one-loop amplitudes. For the latter, one need to address cancelations of various singularities under various limits (such as soft and collinear limits) by combining contributions from various basis. The cancelation of these singularities in a complete loop amplitudes is very intricate. It reflects many important information of the theory under consideration, such as how good (or bad) the divergence will be and if the theory has some unexpected hidden symmetries. It is definitely an important issue and relates to the application in real processes as mentioned in previous paragraph. Although our results in this paper provide a starting point for these discussions, its explicit demonstration will be very complicated and deserves to be an independent

work.

Thirdly, for coefficients of boxes, triangles and bubbles, there are many terms, thus there are many different ways to write down the sum. However, we want to emphasize although there are many different ways to group numerators, the denominators are the same. In other words, the appearance of various second-type singularities is common for all different expressions, especially the highest degrees of second-type singularities are the same. The choice we made here is because we believe this choice gives the best presentation of singularity structure.

Fourthly, as we have mentioned again and again, the coefficients of various bases contain only second-type singularities as classified in [6, 40]. One exception is the singularities for the pentagon as given in $D^{K_i, K_j, K_t, K_\omega, K}$ (Eq.(4.1)). Although it contains the mass, we do not think it belongs to the first-type singularity. This exception is related to the special position of pentagon as a basis in the PV-reduction as we have discussed many times in the paper. What it means or if it is really a singularity deserves further study.

Fifthly, although in this paper, we have identified all singularities. It is still have a lot of work to do to understand their properties. For example, we need to know if they are true singularities for one-loop amplitudes when we sum all together. If they are, where are their locations: on the physical sheet or unphysical sheet. Here we want to distinguish one thing. One of our motivation of current calculations is to find a recursive way to calculate coefficients of various basis. Thus all singularities we found in the paper do contribute coefficients no matter whether they are physical or not or which sheet they locate at. The situation is different from BCFW on-shell recursion relation for tree-level amplitudes where we calculate the complete (global) tree amplitudes thus spurious poles do not give contributions.

Finally, another possible application (which is one of our main motivations) of our results should be mentioned. With Lorentz-invariant forms of coefficients, we can study their factorization property under the various deformation (such as the BCFW-deformation or Risager's deformation [54]). Based on information under deformation, we can try if it is possible to establish some sort of recursion relation.

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A. Sum in spinor form to Lorentz form

In this appendix, we will present a formula which is very important to transform the sum in the spinor form to the Lorentz-invariant form. The typical sum we meet again and again is the following

$$\Sigma_N \equiv \frac{\langle P_1 | T | P_2 \rangle^N}{\prod_{t=1}^N \langle P_1 | Q_t | P_2 \rangle} + \frac{\langle P_2 | T | P_1 \rangle^N}{\prod_{t=1}^N \langle P_2 | Q_t | P_1 \rangle} \quad (\text{A.1})$$

and

$$\Sigma_{N-1}[Q_m] \equiv \frac{\langle P_1|T|P_2\rangle^N}{\prod_{t=1, t \neq m}^N \langle P_1|Q_t|P_2\rangle} + \frac{\langle P_2|T|P_1\rangle^N}{\prod_{t=1, t \neq m}^N \langle P_2|Q_t|P_1\rangle}, \quad \Sigma_1(Q_m) \equiv \frac{\langle P_1|T|P_2\rangle}{\langle P_1|Q_m|P_2\rangle} + \frac{\langle P_2|T|P_1\rangle}{\langle P_2|Q_m|P_1\rangle}. \quad (\text{A.2})$$

where P_1 and P_2 are two null momenta constructed from Q_i and Q_j . Furthermore we suppose i and j are not in the set $\{1, \dots, N\}$ of (A.1). Our derivation of the Lorentz-invariant form will use the inductive method.

A.1 Recursion relation

For a given pair (n, m) simple calculations from (A.2) give

$$\begin{aligned} \Sigma_1(Q_n)\Sigma_{N-1}[Q_n] &= \Sigma_N + \frac{\langle P_1|T|P_2\rangle \langle P_2|T|P_1\rangle \langle P_2|T|P_1\rangle^{N-2}}{\langle P_1|Q_n|P_2\rangle \langle P_2|Q_m|P_1\rangle \prod_{t=1, t \neq n}^{N-1} \langle P_2|Q_t|P_1\rangle} \\ &\quad + \frac{\langle P_2|T|P_1\rangle \langle P_1|T|P_2\rangle \langle P_1|T|P_2\rangle^{N-2}}{\langle P_2|Q_n|P_1\rangle \langle P_1|Q_m|P_2\rangle \prod_{t=1, t \neq n}^{N-1} \langle P_1|Q_t|P_2\rangle} \end{aligned} \quad (\text{A.3})$$

$$\begin{aligned} \Sigma_1(Q_m)\Sigma_{N-1}[Q_m] &= \Sigma_N + \frac{\langle P_1|T|P_2\rangle \langle P_2|T|P_1\rangle \langle P_2|T|P_1\rangle^{N-2}}{\langle P_1|Q_m|P_2\rangle \langle P_2|Q_n|P_1\rangle \prod_{t=1, t \neq m}^{N-1} \langle P_2|Q_t|P_1\rangle} \\ &\quad + \frac{\langle P_2|T|P_1\rangle \langle P_1|T|P_2\rangle \langle P_1|T|P_2\rangle^{N-2}}{\langle P_2|Q_m|P_1\rangle \langle P_1|Q_n|P_2\rangle \prod_{t=1, t \neq m}^{N-1} \langle P_1|Q_t|P_2\rangle}. \end{aligned} \quad (\text{A.4})$$

The sum of Eq. (A.3) and Eq. (A.4) yields

$$\begin{aligned} \Sigma_1(Q_n)\Sigma_{N-1}[Q_n] + \Sigma_1(Q_m)\Sigma_{N-1}[Q_m] &= 2\Sigma_N + \left(\frac{\langle P_1|T|P_2\rangle \langle P_2|T|P_1\rangle}{\langle P_1|Q_n|P_2\rangle \langle P_2|Q_m|P_1\rangle} + \frac{\langle P_1|T|P_2\rangle \langle P_2|T|P_1\rangle}{\langle P_1|Q_m|P_2\rangle \langle P_2|Q_n|P_1\rangle} \right) \\ &\quad \times \Sigma_{N-2}[Q_n, Q_m]. \end{aligned}$$

Using the spinor formulism (remembering P_1, P_2 are two null momenta constructed from Q_i, Q_j), after some trivial manipulations we can get

$$\langle P_1|Q_n|P_2\rangle \langle P_2|Q_m|P_1\rangle + \langle P_1|Q_m|P_2\rangle \langle P_2|Q_n|P_1\rangle = -\frac{8}{Q_i^2}(Q_n|Q_m) \quad (\text{A.5})$$

$$\langle P_1|T|P_2\rangle \langle P_2|T|P_1\rangle = -\frac{4}{Q_i^2}(T|T) \quad (\text{A.6})$$

where we have defined

$$(Q_n|Q_m) \equiv \det \begin{pmatrix} Q_i^2 & Q_i \cdot Q_j & Q_i \cdot Q_n \\ Q_i \cdot Q_j & Q_j^2 & Q_j \cdot Q_n \\ Q_i \cdot Q_m & Q_j \cdot Q_m & Q_n \cdot Q_m \end{pmatrix}. \quad (\text{A.7})$$

So we get the following relation

$$\Sigma_1(Q_n)\Sigma_{N-1}[Q_n] + \Sigma_1(Q_m)\Sigma_{N-1}[Q_m] = 2\Sigma_N + 2 \frac{(T|T)(Q_n|Q_m)}{(Q_n|Q_n)(Q_m|Q_m)} \Sigma_{N-2}[Q_n, Q_m] \quad (\text{A.8})$$

Summing over all pairs (n, m) of (A.8) we get

$$(N-1) \sum_{t=1}^N \Sigma_1(Q_t) \Sigma_{N-1}[Q_t] = N(N-1) \Sigma_N + 2 \sum_{1 \leq t < k \leq N} \frac{(T|T)(Q_k|Q_t)}{(Q_k|Q_k)(Q_t|Q_t)} \Sigma_{N-2}[Q_k, Q_t] \quad (\text{A.9})$$

or

$$\Sigma_N = \frac{1}{N} \left(\sum_{t=1}^N \Sigma_1(Q_t) \Sigma_{N-1}[Q_t] - \frac{2}{N-1} \sum_{1 \leq t < k \leq N} \frac{(T|T)(Q_k|Q_t)}{(Q_k|Q_k)(Q_t|Q_t)} \Sigma_{N-2}[Q_k, Q_t] \right) \quad (\text{A.10})$$

A.2 Proof by inductive method

With some calculations, we find the explicit expression of Σ_N to be

$$\begin{aligned} \Sigma_N = & \frac{1}{\prod_{k=1}^N (Q_k|Q_k)} \left(2^N \prod_{j=1}^N (T|Q_j) \right. \\ & \left. + \sum_{m=1}^{[N/2]} \frac{(-1)^m 2^{N-m} m! (N-2m)! A_{N,m} (T|T)^m}{N!} \sum_{m \text{ pairs } p=1}^m \prod (Q_{p_1}|Q_{p_2}) \prod_{q \in \{N\} - \{m \text{ pairs}\}}^N (Q_q|T) \right). \end{aligned} \quad (\text{A.11})$$

where the notation $[N/2]$ means to take the maximum integer equal to or less than $N/2$, and

$$A_{n,m} = \begin{cases} A_{n-1,m} + A_{n-2,m-1}, & 2m < n \\ 2, & 2m = n \\ 0, & 2m > n \end{cases} \quad (\text{A.12})$$

The second sum at the second line of (A.11) is over all different choices of m pairs in the set $\{1, 2, \dots, N\}$ and each pair contributes a factor $(Q_{p_1}|Q_{p_2})$. After m pairs having been chosen, each remaining element will contribute a factor $(Q_q|T)$. First few examples $N = 1, 2, 3$ can be calculated directly as

$$\begin{aligned} \Sigma_1 &= \frac{\langle P_1|T|P_2 \rangle}{\langle P_1|Q_1|P_2 \rangle} + \frac{\langle P_2|T|P_1 \rangle}{\langle P_2|Q_1|P_1 \rangle} = 2 \frac{(T|Q_1)}{(Q_1|Q_1)}, \\ \Sigma_2 &= 2^2 \frac{(T|Q_1)(T|Q_2)}{(Q_1|Q_1)(Q_2|Q_2)} - 2 \frac{(T|T)(Q_2|Q_1)}{(Q_1|Q_1)(Q_2|Q_2)}, \\ \Sigma_3 &= \frac{1}{(Q_1|Q_1)(Q_2|Q_2)(Q_3|Q_3)} (2^3 (T|Q_1)(T|Q_2)(T|Q_3) - 2(T|T)(Q_2|Q_1)(T|Q_3) \\ &\quad - 2(T|T)(Q_3|Q_1)(T|Q_2) - 2(T|T)(Q_3|Q_2)(T|Q_1)), \end{aligned}$$

which are the same as given by (A.11).

We will prove the formula (A.11) by showing that it satisfies the relation Eq. (A.10) by inductive method. We check this term by term. For the first term of Eq.(A.11), it satisfies the relation Eq. (A.10) obviously since only the first term of Eq. (A.10) contributes. For the second part of the formula (A.11) with given m pairs in the set $\{1, 2, \dots, N\}$, both terms of Eq. (A.10) will contribute. To simplify our

discussion, we use the set $\mathcal{M} = \{m \text{ pairs}\}$ and the set $\mathcal{Q} = \{N\} - \mathcal{M}$. The contribution from the first term of Eq. (A.10) is given by

$$\begin{aligned} T_1 &= \frac{(-1)^m 2^{N-1-m} m! (N-1-2m)! A_{N-1,m} (T|T)^m}{N \prod_{k=1}^N (Q_k|Q_k) (N-1)!} \prod_{p \in \mathcal{M}} (Q_{p_1}|Q_{p_2}) \sum_{q \in \mathcal{Q}} (T|Q_q) \prod_{\tilde{q} \in \mathcal{Q}-q} (Q_{\tilde{q}}|T) \\ &= \frac{(-1)^m 2^{N-1-m} m! (N-1-2m)! A_{N-1,m} (T|T)^m}{N \prod_{k=1}^N (Q_k|Q_k) (N-1)!} \prod_{p \in \mathcal{M}} (Q_{p_1}|Q_{p_2}) (N-2m) \prod_{q \in \mathcal{Q}} (Q_q|T). \end{aligned}$$

The sum in the first line of T_1 comes from choosing which $q \in \mathcal{Q}$ belongs to the Σ_1 part. The contribution from the first term of Eq. (A.10) is given by

$$\begin{aligned} T_2 &= - \frac{(-1)^{m-1} 2^{N-m-1} (m-1)! (N-2m)! A_{N-2,m-1} (T|T)^m}{N(N-1) \prod_{k=1}^N (Q_k|Q_k) (N-2)!} \prod_{q \in \mathcal{Q}} (Q_q|T) \sum_{p \in \mathcal{M}} (Q_{p_1}|Q_{p_2}) \prod_{\tilde{p} \in \mathcal{M}-p} (Q_{\tilde{p}_1}|Q_{\tilde{p}_2}) \\ &= - \frac{(-1)^{m-1} 2^{N-m-1} (m-1)! (N-2m)! A_{N-2,m-1} (T|T)^m}{N(N-1) \prod_{k=1}^N (Q_k|Q_k) (N-2)!} \prod_{q \in \mathcal{Q}} (Q_q|T)^m \prod_{\tilde{p} \in \mathcal{M}} (Q_{\tilde{p}_1}|Q_{\tilde{p}_2}). \end{aligned}$$

The sum in the first line of T_2 comes from choosing which pair $p \in \mathcal{M}$ does not belong to the Σ_{N-2} part. Summing T_1 and T_2 , with a little algebra, we can see that it reproduces the corresponding terms of formula (A.11).

A special case of the above proof is that when $N = 2m$, only the second term of Eq. (A.10) contributes. It is easy to see that we do have $A_{2m,m} = A_{2m-2,m-1} = 2$ as given by (A.12).

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